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Modeling a fish population with diffusive and advective movement in a spatial environment

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To the Graduate Council:

I am submitting herewith a dissertation written by Qingping Deng entitled "Modeling a fish population with diffusive and advective movement in a spatial environment." I have examined the final electronic copy of this dissertation for form and content and recommend that it be accepted in partial fulfillment of the requirements for the degree of Doctor of Philosophy, with a major in Mathematics.

Thomas G. Hallam, Major Professor

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To the Graduate Council:

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MODELING A FISH POPULATION WITH DIFFUSIVE AND ADVECTIVE MOVEMENT IN A SPATIAL ENVIRONMENT

A Dissertation
Presented for the
Doctor of Philosophy
Degree
The University of Tennessee, Knoxville

Qingping Deng
May 2000

獻給我的全家

To My Family

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Abstract

This dissertation has developed an individual-based, physiologically structured model for a fish population with diffusive and advective movement in a spatial environment. It incorporates spatio-temporal processes and individual processes simultaneously into the population dynamic model of a McKendrick-von Foerster type partial differential equation. An individual fish is physiologically structured according to age, lipid and structure (protein and carbohydrates). Fish are assumed to be immobile in their embryonic stage and the fish begin to feed and might move after the embryonic stage. Advective processes are induced by environmental heterogeneity, in which fish move toward neighboring areas with different levels of, for instance, resource density or/and chemical toxicant concentration. The population dynamic model is complicated, in that it is a mixed type partial differential equation that combines a quasi-linear hyperbolic equation in the embryonic stage and a degenerate parabolic equation in the older life stage.

Some mathematical aspects of the model of primary interest have been discussed. The existence of a local weak solution has been shown. By the constructive analysis used to demonstrate the existence of a local solution, a computational scheme for the mathematical model has been developed. For the individual growth model, we simply use the implicit Runge-Kutta method. For the population dynamic model of a partial differential problem, we use a characteristic finite difference method in the age-time domain and a finite element method with numerical integration and upwind modification in the spatial domain. Furthermore, the numerical scheme has been proved to yield numerical approximations with optimal error estimates and produce biologically reasonable approximate solutions as well.

The mathematical and computational models have been used to study a specific model of a population of rainbow trout, *Oncorhynchus mykiss*, in a spatial environment. We have investigated numerically the dynamics of spatio-temporal population distribution variations as they are viewed through the fish population density, total fish biomass, total fish age, total fish lipid, total fish structure (protein) and total fish protected protein. Furthermore, the model has also been used to study the effects of a spatially distributed nonpolar narcotic chemical on a rainbow trout population. The combined effects of lethal and sublethal toxicant effects have been considered.

The methodologies and conclusions in this dissertation can be extended immediately into other populations and even some community settings, such as the fish–*Daphnia* predator–prey model if *Daphnia* are assumed to be immobile.

Contents

Overview **1**

1 Introduction and Preliminaries **8**

1.1 Fish Individual Model 10

1.2 Population Dynamic Models 16

1.3 Temperature and Dissolved Oxygen Effects 23

1.4 Chemical Toxicant Effects 25

1.5 Individual-Based Population Models 32

2 Mathematical Models for Individual-Based Populations **40**

2.1 Mathematical Derivations 42

2.2 Age Structured Population Dynamic Problems 50

2.3 Mathematical Treatments 83

3 Computational Techniques for an Individual-Based Population Model **91**

3.1 Numerical Methods for Ordinary Differential Problems 93

3.2 Numerical Schemes for Population Models 96

3.2.1 Numerical Scheme for Age structured Population Problem (I) 97

3.2.2 Numerical Scheme for Age structured Population Problem (II) 106

3.2.3 Numerical Scheme for Age structured Population Problem (III) 140

3.3 Numerical Scheme for Mathematical Models of Individual-Based Populations 153

3.4 Computational Model and Algorithm Aspects 167

3.5 A Parallel Procedure for the Linear Systems 172

4 Modeling a Fish Population in a Spatial Environment 184

4.1 Introduction 185

4.2 A Physiologically–Based Fish Individual Model 187

4.3 Fish Population Dynamics 189

4.4 Numerical Computation Procedure 194

4.5 Numerical Experiments 199

4.6 Discussion and Future work 203

5 Modeling Toxicant Effects on a Fish Population in a Spatially

Heterogeneous Environment **204**

5.1 Introduction 205

5.2 Exposure–Effect Model 207

5.3 Individual-Based Population Model and Its Numerical Scheme . . 212

5.4 Effects of Toxicant on Population 220

5.5 Discussion and Further Work 224

Bibliography **226**

Appendix **244**

Vita **287**

List of Tables

1 Parameter values and units in the individual model (I) 245
2 Parameter values and units in the individual model (II) 246
3 The variables and parameters in the uptake model 247

List of Figures

1 Individual Based Adult Fish Model 248

2 Individual Fish Growth (1) 249

3 Individual Fish Growth (2) 250

4 Relationship between $\log LC_{50}$ and $\log K_{ow}$ 251

5 Flow Chart for Computational Model 252

6 Double Linked List of *q-cohort* 253

7 Dequeue Structure of *Age-Group* 254

8 Resource Distribution Patterns 255

9 Total Fish Number of *Case 4.1* 256

10 Population Dynamics/Distribution at a Location/Time of *Case 4.1* 257

11 Total Biomass Distribution of *Case 4.1* 258

12 Total Age Distribution of *Case 4.1* 259

13 Total Lipid and Protein Distribution of *Case 4.1* 260

14 Total Protected Protein Distribution of *Case 4.1* 261

15 Total Fish Number of *Case 4.2* 262
16 Population Dynamics/Distribution at a Location/Time of *Case 4.2* 263
17 Total Biomass Distribution of *Case 4.2* 264
18 Total Lipid and Protein Distribution of *Case 4.2* 265
19 Total Age and Protected Protein Distribution of *Case 4.2* 266
20 Total Fish Number and Biomass Distribution of *case 4.3* 267
21 Population Dynamics/Distribution at a Location/Time of *Case 4.3* 268
22 Total Lipid and Protein Distribution of *Case 4.3* 269
23 Total Age and Protected Protein Distribution of *Case 4.3* 270
24 Total Fish number and Biomass Distribution of *Case 4.4* 271
25 Total Lipid and Protein Distribution of *Case 4.4* 272
26 Total Age and Protected Protein Distribution of *Case 4.4* 273
27 Resource and Chemical Distribution 274
28 Total Fish Number and Biomass Distribution of *Case 5.1* 275
29 Total Lipid and Protein Distribution of *Case 5.1* 276
30 Total Age and Protected Protein Distribution of *Case 5.1* 277
31 Total Fish Number and Biomass Distribution of *Case 5.2* 278
32 Total Lipid and Protein Distribution of *Case 5.2* 279
33 Total Age and Protected Protein Distribution of *Case 5.2* 280
34 Total Fish Number and Biomass Distribution of *Case 5.3* 281
35 Total Lipid and Protein Distribution of *Case 5.3* 282

36 Total Age and Protected Protein Distribution of *Case 5.3* 283

37 Total Fish Number and Biomass Distribution of *Case 5.4* 284

38 Total Lipid and Protein Distribution of *Case 5.4* 285

39 Total Age and Protected Protein Distribution of *Case 5.4* 286

Overview

Individual-based, physiologically structured models of ecosystems (populations and communities) in a homogeneous environment have been an important area for many years (cf. [45, 49, 54, 70, 71]). This type of model often consists of 1) an energetics based growth model for each type of individual organism, including physical and stresses that impact individual organisms; 2) each population represented by appropriate physiological variables through a McKendrick-von Foerster type partial differential equation which incorporates the dynamics of the individuals (cf. [17, 54, 82, 89]); and 3) the appropriate population models are combined through inter-specific interactions to form the community model (cf. [17, 44, 54, 82]) . However, the development of individual-based structured ecosystems in a heterogeneous environment is still in its infancy, in spite of the fact that most natural environments are heterogeneous, especially, in spatial structure. In heterogeneous environments, an important aspect of natural populations is the structural variation which arises from differences in individuals and environmental heterogeneities as well. This structural variability is compounded when spatio-temporal processes and their influence on population dynamics is considered. In particular, spatial structure and physical movements of individuals arise because of the environmental heterogeneity. In this dissertation, we develop an individual-based, physiologically structured population model in a heterogeneous environment with different levels of food density or/and chemical toxicant concentration. Spatio-temporal processes incorporates simultaneously into the population dynamic of a McKendrick-von Foerster type partial differential equation. Diffusive and advective movements have been introduced into the population dynamics represented by McKendrick-von Foerster type partial differential equations. By an advective process, we mean movement of individuals towards neighboring areas with preferential quality, for instance, the areas where food resource density is higher and/or chemical toxicant density is lower.

This dissertation mainly focuses on the development and implementation of individual based, physiologically structured fish population models with diffusive and advective movements in heterogeneous spatial environments. However, the methodology and conclusions can be extended immediately to other populations and even some communities. Results apply to a fish–*Daphnia* predator–prey model if *Daphnia* are assumed to be immobile, perhaps a good initial approximation, since their movement is small, relative to fish movement.

Chapter 1 covers introductory materials. The rest of this dissertation is composed of four chapters, which discuss mathematical models and analyses, numerical techniques and schemes, implementation and analysis of a model of a fish population with diffusive and advective movements in a natural spatial environment, and implementation and analysis of a model containing toxicant effects on a fish population whose individuals are influenced by both diffusive and advective movement processes, respectively.

Chapter 2 presents some mathematical results for individual-based, physiologically structured population models in a heterogeneous spatial environment, where the individuals are assumed immobile at the embryonic stage and are subject to both diffusion and advection in the rest of their life period. A mathematical derivation of the population model as a partial differential equation is given. The mathematical formulation of the model is a nonlocal initial-boundary value problem of a nonlinear partial differential equation with discontinuous coefficients coupled with an initial value problem of a ordinary differential system. The existence of a local weak solution of the mathematical model problem is shown. The basic idea of our mathematical analysis is from the method of compactness in functional analysis. The analysis is based on a localization technique, an unstructuralization technique for physiological structures, and a linearization technique. We first localize the original problem. That is, we introduce a small positive parameter $\Delta t > 0$ and split the original mathematical problem into a sequence of local problems over the small time interval $[t_i, t_{i+1}]$ $(t_{i+1} = t_i + \Delta t, \ i = 0, 1, \cdots)$.Then, for each local problem, we will separately consider the ordinary differential system of the individual growth model and the partial differential problem of the population dynamic model. More precisely, we first solve the initial value problem of the ordinary differential system for the individual-based model and then plug the solution of the ordinary differential system into the partial differential problem of the population dynamic model. Then we only need solve a partial differential problem for an age structured population over the small time interval. In other words, we unstructure the physiological structures in the population dynamic model of the original mathematical system in local small time intervals. Therefore, we can obtain an approximate solution for the local problem, as well as an approximate initial-boundary condition for the local problem over the next small time interval. Moreover, we put these approximate solutions of local problems together to form an approximate solution for the original mathematical model problem. However, the induced local age structured population mathematical model is also not easy to solve since it is still a nonlocal initial-boundary value problem of nonlinear partial differential problem with discontinuous coefficients. To solve this kind of partial differential problem for the age structured population, we linearize it by using the technique involving a positive delay to overcome the nonlinearity and then applying a technique of fixed point theory to the related partial differential problem involving an integral equation in its nonlocal initial-boundary conditions. These analysis strategies and conclusions provide the motivation and foundation to construct the numerical approximation schemes in Chapter 3. As a basis and preparation of the analysis, we first discuss three related auxiliary age-structured population dynamic models. In fact, as by-products, many of these results for auxiliary problems are also significant as partial differential equation problems.

Chapter 3 considers some computational aspects of the models formulated in

Chapter 2. The basic idea to construct the numerical scheme is motivated by the strategy of mathematical analysis developed in Chapter 2, that is, the localization technique, the unstructuralization technique for the physiological structures, and the linearization technique. For the ordinary differential system problem for the individual model, we use the implicit Runge-Kutta method due to stiffness. For the partial differential equation problem associated with the population dynamics, we use a characteristic finite difference discretization in the age-time domain and a finite element method with numerical integration and upwind modification of advective terms in the spatial domain. To do some numerical analysis, we also develop and analyze the numerical approximate schemes for the three auxiliary age structured population dynamic models of Chapter 2. The analyses have shown that the numerical schemes not only have optimal error estimates from the perspective of numerical analysis, but they also always produce biologically reasonable approximate solutions. Finally, we discuss the computing and coding methodology for implementing the numerical scheme. As a very important related problem, we give a parallel procedure for solving large linear systems such as one obtained from our computational model, which is the core of the numerical implementation of the computational model.

In Chapter 4, we apply the mathematical and computational model to dynamics of a fish population in a bounded linear habitat in which the fish can have diffusive and advective movements. The fish population is structured according to the physiological variables age, lipid, and structure (protein and carbohydrates) and so an individual model, described as an ordinary differential system, is needed to model the growth of those physiological variables. The individual model has been developed to deal with rainbow trout, *Oncorhynchus mykiss*, and is based on energy budget techniques. The movement behavior of the fish is a function of the physiological state of the individual. The fish is assumed to be immobile at the embryonic stage and may have diffusive and advective movements in the rest of life period. Diffusion is a kind of random dispersal or random walk plus density-dependent dispersal so that the local flow of the population lies in the direction of decreasing density of fish. Advection assumes the fish moves towards the location where the resource density is higher if its energy gained is less than energy demanded. More precisely, the advective movement is determined by the gradient of food resource density and whether the energy gained exceeds the energy demand. The development and discussion will focus on the spatio-temporal aspects of the population dynamics.

In Chapter 5, we investigate the chemical toxicant effects on a fish population in a spatially heterogeneous toxicant environment. We apply the models developed in Chapter 2, 3 and 4 to a fish population in a bounded linear habitat with heterogeneous chemical toxicant levels and food resource levels. We only consider a simple diffusive process – random walk dispersal. The advective process is more complicated than that in Chapter 4 since individuals may alter their movement in response to changes in not only resource density, but to changes in the concentration of contaminated media as well. In addition, exposed organisms may avoid contaminated media, may be attracted to contaminated resource (e.g. pesticide-debilitated prey) or may lose their ability to detect contamination due to toxic effects. If the individual does not have the ability to detect contamination, we assume that there is no advective movement induced by chemical toxicant. As in Chapter 4, the advective movement induced by food resource heterogeneity is determined by the gradient of food resource density and whether the energy gained exceeds the energy demands. The advective movement induced by chemical toxicant is determined by the gradient of toxicant concentration as well as whether an individual avoids contaminated media or is attracted to contaminated media. The chemical exposure might occur through the environmental and/or the food pathways. Like Chapter 4, the development and analysis focus on the spatio-temporal aspects of population dynamics. We demonstrate that spatial heterogeneity can influence the physiological structure of the population and determine the survival or extinction of the population. Effects depend on the spatial pattern of the toxicant and resource, as related to the distribution of individuals in space, during the exposure.

Chapter 1

Introduction and Preliminaries

Natural environments are usually heterogeneous from many perspectives including spatial structure. In natural populations and communities, individuals of different age, size and other physiological variables display differences in growth, movement, and behavior, and individuals of the same age, size and other physiological variables can display different responses in different environments. These differences among individuals within a population, which may be due to demographic, genetic or environmental processes, often force consideration of an individual-based approach instead of an aggregated one when a more faithful ecological representation is desired. For the most part, environmental variables, such as chemicals or temperature, affect the physiological and behavioral processes of individuals, and, subsequently impact the behavior of the population as a whole. After the effects on the physiological processes at the individual level have been assessed and the individuals all combined to form a population, the study of the dynamics of the population is viable. Therefore, in a heterogeneous environment, an individual-based model is usually important to study environmental effects at the population or community level.

In this thesis, we have developed and analyzed the mathematical and computational models of an individual-based, physiologically structured population of fish in spatially heterogeneous chemical toxicant environment, and implement computational simulation schemes for some typical cases. The mathematical models are described as a partial differential equation problem coupled with an ordinary differential system to model an individual-based fish population with diffusion and advection in a heterogeneous spatial chemical toxicant environment. More precisely, an initial value problem of an ordinary differential system is used to describe the growth of individual fish; a nonlocal initial-boundary value problem of a partial differential equation with discontinuous coefficients is used to describe the fish population dynamics and distribution, in particular, including reproductions and movements. Some mathematical analyses for the individual-based fish population mathematical models are presented. Then, the computational models for individual-based fish populations by using the mathematical models are constructed. Moreover, some considerations of the convergence analyses and aspects for the numerical approximate schemes are shown. Finally, the mathematical and computational models are applied to simulate a fish population in a heterogeneous closed bounded environment and toxicant effects on a fish population in a heterogeneous chemical environment, where the combined chemical toxicant effects of lethal and sublethal effects are considered.

In the rest of Chapter 1, some preliminary materials including individual fish growth models, basic population dynamic models, models for temperature and dissolved oxygen effects, models for chemical toxicant effects and the individual-based fish population mathematical models are presented.

1.1 Fish Individual Model

The individual-based model we use for the dynamics of an individual fish is based on the physiological-based individual model introduced by Hallam *et al* [45, 47]. It has been parameterized for rainbow trout, *Oncorhynchus mykiss*. However, because of the generality of the energetics approach (cf. [70, 71]), it can be used for other species of fish with some modifications. We here provide a brief description of fish individual model, which is summarized from [45, 47]. The mathematical individual-based fish model employed in [45, 47] is based on the energetics of an individual female fish (see Figure 1 [1]). Each organism is composed of two major components, lipid m_L (g) and structure, m_S (g) (protein and carbohydrates). Each of these components consists of a labile and nonlabile portion. The non-

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[1] All Tables and Figures appear in Appendix

labile portion is the mass of lipid and structure bound in somatic tissue that cannot be mobilized even under condition of starvation. The labile portion of lipid and structure is available for growth and reproduction. The dynamics of individual fish are represented by an ordinary differential equation system which gives the rates of change of the mass of lipid and structure.

$$\begin{aligned} \frac{dm_L}{da} &= g_L \equiv G_L - F_L \\ \frac{dm_S}{da} &= g_S \equiv G_S - F_S, \end{aligned} \tag{1.1}$$

where G_L and G_S represent the growth of lipid and structure, respectively; and F_L and F_S represent the loss of lipid and structure, respectively. These rates are determined by the difference in the inputs and the outputs. The inputs are represented by the growth of the lipid and structure compartments whereas the outputs are the losses from the compartments. The growth of lipid and structure of a fish (measured by the assimilated lipid and structure) is obtained from feeding on a constant level of resource which also has lipid and structure components, the densities of which are denoted by x_L (g/cm^3) and x_S (g/cm^3). The amount of resource that can be converted to viable energy is based on the assimilation efficiencies of the lipid and structure, represented by A_{0L} $(nondim)$ and A_{0S} $(nondim)$ in the model. The losses represent lipid and structure matter allocation to egg production, energy allocation to maintenance, specific dynamic action, activity (including diffusion, advection etc.) and reproduction. The losses due to maintenance, specific dynamic action, and activity occur on a continuous time scale and reproductive losses occur periodically on a discrete time scale.

The life history of a female fish is followed from the deposition and fertilization of the eggs to when the fish eventually dies. There are two sets of ordinary differential equation systems describing two stages in the life of a fish. The first set is for the growth during the embryonic stage. The dynamics of lipid and structure mass of an individual fry (young trout before it starts feeding) are represented only by the cost of differentiation and maintenance, which is assumed to be proportional to the size of the components, and are modeled by the following equations:

$$\begin{aligned} \frac{dm_L}{da} &= -B_1 m_L \\ \frac{dm_S}{da} &= -B_2 m_S \end{aligned} \tag{1.2}$$

where B_1 and B_2 are the compartmental rate coefficients in units of $(1/d)$; and with the initial condition

$$\begin{aligned} m_L|_{a=0} &= m_{L_0} \\ m_S|_{a=0} &= m_{S_0} \end{aligned} \tag{1.3}$$

where m_{L_0} and m_{S_0} are the initial lipid and structure content of an agg. Rainbow trout eggs hatch 34-36 days after fertilization at 10^oC (cf. [103]), the yolk sac is depleted 3-7 days later, and fry begin feeding about 51 days after hatching (cf. [99]). So, in the embryonic stage, they actually decrease in size.

The fry begin to feed after the embryonic stage. This is the second stage in the life of the organism and there is a new set of ordinary differential equations to describe the growth process. The dynamics of the lipid and structure mass are modeled by the following equations:

$$\frac{dm_L}{da} = \frac{A_{0L}X_L}{X}F - \begin{cases} A_3(m_L - \epsilon m_{PS}) & \text{for } D > E \\ A_3(m_L - \epsilon m_{PS})\dfrac{D}{E} & \text{for } D \leq E \end{cases} \tag{1.4}$$

$$\frac{dm_S}{da} = \frac{A_{0S}X_S}{X}F - \begin{cases} A_4(m_S - m_{PS}) & \text{for } D > E \\ A_4(m_S - m_{PS})\dfrac{D}{E} & \text{for } D \leq E \end{cases} \tag{1.5}$$

where the initial conditions are given by the terminal conditions from the embryonic stage equations (1.2) and (1.3) m_L, m_S, A_{0L}, A_{0S}, X_L, X_S are defined as previously; m_{PS} is the mass of protected structure, which is assumed to be nondecreasing with age and is computed as a fraction βm_S of the structural mass, for example, $m_{PS} = \max(\beta\, m_S,\ m_{PS})$.

In the growth terms of (1.4) and (1.5), $X = X_L + X_S$ (g) represents the resource and F (g/d) represents the feeding rate of an individual, which is governed by constraints. The constraints are imposed by processes associated with encounter, pursuit and digestion of a prey. These processes are implemented sequentially, i.e., the encounter, pursuit and digestion of a prey must be completed first before another prey may begin to be processed. For a sequential process, the feeding rate is given by the form (cf. [55])

$$F = \frac{1}{T_e + T_p + T_d} \,. \tag{1.6}$$

The terms in the denominator represent the characteristic times (d/g) for encounter, pursuit, and digestion of prey. Therefore, $\frac{A_{0L}X_L}{X}F$ and $\frac{A_{0S}X_S}{X}F$ represent the mass of lipid and the mass of structure gained by consumption per unit time. For a single predator feeding upon a single prey, F can be given by

$$F = \frac{1}{[a_d X]^{-1} + \frac{s_d}{M_p \delta_v} + [k M_g]^{-1}} \,.$$

In the loss terms of (1.4) and (1.5), the terms $(m_L - \epsilon m_{PS})$ (ϵ is nondimensional: mass of lipid/mass of structure) and $(m_S - m_{PS})$ represent the labile portions of lipid and structural mass of an individual. E denotes the energetic equivalent of the mass that an individual utilizes in order to maintain basal metabolism. This energy is derived from the labile lipid and labile structure using the function

$$E = 3.768 \cdot 10^4 A_3 (m_L - \epsilon m_{PS}) + 1.675 \cdot 10^4 A_4 (m_S - m_{PS}) \,,$$

where A_3 and A_4 are the rates $(1/d)$ at which lipid and structure are mobilized to maintain basal metabolism, and the numbers in each term are the energetic values in *joules* of 1 g of lipid and structure, respectively. The rates at which the labile lipid and structure are utilized depend on the energy demands, D, of the organism. This is accomplished via supply energy that is apportioned by the fraction D/E. The total energy demand, D, is comprised of a number of subcomponents: maintenance, specific dynamic action which represents work associated with feeding, and activity which represents the work associated with swimming.

The growth of each organism is described in equations (1.2) - (1.3) and (1.4) - (1.5) until reproduction occurs after the maturation size is reached and age is 1 year or older. At the time when reproduction occurs, discrete losses of labile lipid and structure associated with reproduction are subtracted from m_L and m_S. The organism then begins to grow again according to (1.4) - (1.5) with the initial conditions on m_L and m_S reset to the values after the reproductive losses have occurred. This process is repeated periodically, with reproduction occurring every year as long as the organism has sufficient lipid and structure to produce eggs and the energy required from the reproduction processes, until death occurs.

For more details about the definitions, we refer to Hallam *et al* [47, 45]. Table 1 and Table 2 in Appendix summarize the model parameters and gives the default values used in the simulations.

1.2 Population Dynamic Models

This section discusses mathematical formulations of individual-based fish population models. We assume that ρ represents the population density function, a represents *age* and t represents *time*. If fish live in a homogeneous environment and do not make any spatial movements, then the fish population dynamic model is the following *extended McKendrick-von Foerster equation* (cf. [17, 70]):

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial a} + \frac{\partial(\rho\, g_L)}{\partial m_L} + \frac{\partial(\rho\, g_S)}{\partial m_S} = -\mu\rho \tag{1.7}$$

where μ $(1/d)$ is the mortality rate. Clearly, (1.7) is a hyperbolic partial differential equation. As is well-known, in addition to the partial differential equation (1.7), we need to adjoin the initial conditions

$$\rho(0, a, m_L, m_S) = \rho_0(a, m_L, m_S) \tag{1.8}$$

and also need the boundary condition, which is called the *renewal equation*,

$$\rho(t, 0, m_{L_0}, m_{S_0}) = \int_0^{A_m}\int_0^{\infty}\int_0^{\infty} \beta\rho(t, a, m_L, m_S)\, da\, dm_L\, dm_S\ , \tag{1.9}$$

where A_m is the maximum age; and β the reproduction rate, represents the expected number of eggs with lipid content m_{L_0} and structure content m_{S_0} born to an individual of age a with lipid content m_L and structure content m_S at time t.

The *renewal equation* (1.9) describes the birth process mathematically.

If fish live in a heterogeneous spatially environment and can make diffusive and advective movements, then the fish population dynamic model is another *extended McKendrick-von Foerster equation* (cf. [17, 70]) as follows:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial a} + \frac{\partial (\rho\, g_L)}{\partial m_L} + \frac{\partial (\rho\, g_S)}{\partial m_S} - \nabla \mathcal{D} = -\mu \rho\,. \tag{1.10}$$

where $\nabla = \nabla_x$, x represents the spatial position, $\mathcal{D}$ is the flux of ρ, which can have several forms, in particular, the following form will be the focus in this thesis

$$\mathcal{D} = k\, \nabla \rho - \mathbf{q}\, \rho \tag{1.11}$$

(1.11) represents a diffusive and advective movement. Indeed, we mostly consider the simpler diffusion as follows:

$$\mathcal{D} = k\, \nabla \rho \tag{1.12}$$

However, all the related results and methods can be applied to other cases with both diffusion and advection, such as (1.11). This is because, mathematically, the partial differential equation (1.10) with $\mathcal{D}$ in (1.11) can be easily rewritten the equation (1.10) with $\mathcal{D}$ in (1.12) in a new μ. Clearly, (1.10) is a degenerate parabolic partial differential equation. We assume that fish live in a bounded connected domain $\Omega \subset \mathcal{R}^{\mathbf{n}}$ ($\mathbf{n} = 1, 2, 3$), with the boundary $\partial\Omega$. Similarly as before, in addition to the partial differential equation (1.10), we need to adjoin the initial conditions

$$\rho(0, a, m_L, m_S, x) = \rho_0(a, m_L, m_S, x) \, , \tag{1.13}$$

and a spatial boundary condition such as

$$\mathcal{D} \cdot \nu = 0 \quad or \quad \rho = 0, \quad \text{on} \quad \partial\Omega \, , \tag{1.14}$$

where ν is the unit outward normal direction of $\partial\Omega$. The boundary condition asserts that there is no flow of the population across the boundary of the habitat or no fish on the boundary, and the birth boundary condition or renewal equation

$$\rho(t, 0, m_{L_0}, m_{S_0}, x) = \int_0^{A_m} \int_0^{\infty} \int_0^{\infty} \beta \rho(t, a, m_L, m_S, x) \, da \, dm_L \, dm_S \, , \tag{1.15}$$

where β is the reproduction rate.

Furthermore, we now consider the third case which is more complicated and can be regarded as a combination of the population dynamic model (1.7) and (1.10). In this case, fish are assumed to live in a heterogeneous bounded spatial environment, to be immoble in their embryonic stage $[0, J]$ and might have diffusive and advective movements in the older life stage $(J, A_m]$. Therefore, we develop the population dynamic model by simply combining (1.7) and (1.10) together. That is, we use the population dynamic model (1.7) in the embryonic stgae $[0, J]$ and (1.10) in the older life stage $(J, A_m]$. Thus, we can write the population dynamic model as follows:

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial a} + \frac{\partial(\rho\, g_L)}{\partial m_L} + \frac{\partial(\rho\, g_S)}{\partial m_S} &= -\mu\rho \\ &\text{for } \forall\ t \in (0, T], a \in (0, J], x \in \Omega, \end{aligned} \tag{1.16}$$

with the initial and boundary condition

$$\begin{aligned} &\mathcal{D}\cdot\nu = 0 \quad \text{or} \quad \rho = 0, \quad \text{on } \partial\Omega \\ &\rho(0, a, m_L, m_S, x) = \rho_0(a, m_L, m_S, x) \\ &\rho(t, 0, m_{L_0}, m_{S_0}, x) = \int_0^{A_m}\int_0^{\infty}\int_0^{\infty} \beta\rho(t, a, m_L, m_S, x)\, da\, dm_L\, dm_S \end{aligned} \tag{1.17}$$

and

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial a} + \frac{\partial(\rho\, g_L)}{\partial m_L} + \frac{\partial(\rho\, g_S)}{\partial m_S} - \nabla\mathcal{D} &= -\mu\rho \\ &\text{for } \forall\ t \in (0, T], a \in (J, A_m], x \in \Omega, \end{aligned} \tag{1.18}$$

with the initial and boundary condition

$$\begin{aligned} &\mathcal{D}\cdot\nu = 0 \quad \text{or} \quad \rho = 0, \quad \text{on } \partial\Omega \\ &\rho(0, a, m_L, m_S, x) = \rho_0(a, m_L, m_S, x), \\ &\rho(t, J, m_L, m_S, x) \quad \text{determined by (1.16) - (1.17)} \end{aligned} \tag{1.19}$$

Similarily, we mostly consider the flux $\mathcal{D}$ with the forms of (1.11) and (1.12). We now extend k and $\mathbf{q}$ as follows,

$$\tilde{k} = \begin{cases} 0 & \text{if} \quad a \in [0, J] \\ k & \text{otherwise} \end{cases} \tag{1.20}$$

$$\tilde{\mathbf{q}} = \begin{cases} 0 & \text{if} \quad a \in [0, J] \\ \mathbf{q} & \text{otherwise} \end{cases} \tag{1.21}$$

Thus, if $\mathcal{D}$ is defined as (1.11), then we can rewrite the population dynamic model (1.16) – (1.19) as a unified form:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial a} + \frac{\partial (\rho\, g_L)}{\partial m_L} + \frac{\partial (\rho\, g_S)}{\partial m_S} - \nabla \cdot (\tilde{k}\, \nabla \rho - \tilde{\mathbf{q}} \rho) = -\mu \rho \qquad \text{for } \forall\, t \in (0, T], a \in [0, A_m], x \in \Omega. \tag{1.22}$$

with the initial and boundary condition

$$\begin{aligned} &\tilde{k}(\frac{\partial \rho}{\partial \nu} - \tilde{\mathbf{q}} \cdot \nu) = 0 \;\text{ or }\; \rho = 0, \quad \text{on } \partial\Omega \\ &\rho(0, a, m_L, m_S, x) \quad = \rho_0(a, m_L, m_S, x) \\ &\rho(t, 0, m_{L_0}, m_{S_0}, x) = \int_0^{A_m} \int_0^{\infty} \int_0^{\infty} \beta \rho(t, a, m_L, m_S, x)\, da dm_L dm_S \end{aligned} \tag{1.23}$$

If $\mathcal{D}$ is defined as (1.12), the unified form of the population dynamic model

(1.16) – (1.19) can be rewritten as

$$\begin{aligned}&\frac{\partial\rho}{\partial t}+\frac{\partial\rho}{\partial a}+\frac{\partial(\rho\, g_L)}{\partial m_L}+\frac{\partial(\rho\, g_S)}{\partial m_S}-\nabla\cdot(\tilde{k}\,\nabla\rho)=\ -\mu\rho\\&\qquad\qquad\qquad\text{for } \forall\ t\in(0,T], a\in[0,A_m], x\in\Omega.\end{aligned}\tag{1.24}$$

with the initial and boundary condition

$$\begin{aligned}&\tilde{k}\,\frac{\partial\rho}{\partial\nu}=0\ \text{ or }\ \rho=0,\quad\text{on }\partial\Omega\\&\rho(0,a,m_L,m_S,x)\ \ =\rho_0(a,m_L,m_S,x)\\&\rho(t,0,m_{L_0},m_{S_0},x)=\int_0^{A_m}\int_0^{\infty}\int_0^{\infty}\beta\rho(t,a,m_L,m_S,x)\,dadm_Ldm_S\end{aligned}\tag{1.25}$$

Both (1.22) – (1.23) and (1.24) – (1.25) are nonlocal initial-boundary value partial differential equation problems with discontinuous coefficients. They are complicated and hard to be solve. We are not aware of any discussions and analyses about such models. This thesis will analyze and discuss this kind of population dynamic model and apply it into individual-based population models. As we explained before, our mathematical analyses and discussions mostly focus on the problem (1.24) – (1.25) since the problem (1.22) – (1.23) can be easily rewritten as the form of the problem (1.24) – (1.25) with a new μ. However, our numerical simulations and examples are shown for both problem (1.22) – (1.23) and problem (1.24) – (1.25).

We now give a brief discussion about the reproduction and mortality. Fish are assumed to reproduce almost periodically after attaining maturation size (Brown

[10] indicates that seasonal periodicity in egg production is characteristic of many fish species). More precisely, we assume that fish 365 days old or older reproduce once in a fixed time period (365 days in our computations) in a specific time window. Reproduction occurs in a time window to represent seasonal aspects of reproduction. The organism grows according to equations (1.2) - (1.3) and (1.4) - (1.5) until reproduction occurs in the first reproductive window at the minimum adult age J. At this time, losses associated with reproduction are computed, and the initial conditions of (1.4) - (1.5) are reset. The individual again grows according to (1.4) - (1.5) until it may reproduce again in the same time window of next year if it can meet all other physiological requirements. This process is repeated as an almost periodical event until the individual dies. An organism dies either because it reaches the prescribed maximum age or because its structural mass, m_S, decreases below the protected structural mass m_{PS}. The latter may happen due to losses associated with reproduction and/or due to shortage of food.

Losses associated with reproduction represent lipid and structural mass needed for egg formation as well as the energy utilized to accomplish this transfer of mass. These allocations obviously do not occur instantaneously. Because there is little specific information on the time scales of these processes and they are short relative to population time scales, we treat them as discrete events.

The number of eggs produced by an individual will be constrained by both lipid and structural mass available for reproduction. Although variation in egg size is probably controlled by many factors, we assume here that only lipid constrains this process. Therefore, the egg is assumed to be composed of a fixed amount of structural material and a variable amount of lipid. The governing factors for allocation of lipid to eggs are assumed to be labile lipid, $m_L - \epsilon m_{PS}$, and a counteractive coupling with labile structure. The computational formula for the number of eggs and their lipid amount can be found in Hallam *et al* [47, 45].

The mortality function μ is assumed to have the form (cf. [47])

$$\mu = \mu_a + \mu_w + \mu_y + \mu_d, \tag{1.26}$$

where μ_a represents the mortality in the population due to age, μ_w represents weight-dependent mortality, μ_y represents the mortality to the young of the year and μ_d represents a density dependent mortality. For their compuational formula, we refer to [47, 45].

Table 1 and Table 2 in Appendix summarize the model parameters and gives the default values used in the simulations.

1.3 Temperature and Dissolved Oxygen Effects

This section introduces the effects of temperature and dissolved oxygen on fish population dynamics. The individual-based fish population models of the last two sections are modified to include the effects of change in temperature and concentration of dissolved oxygen. Effects of both temperature and dissolved oxygen occur on three physiological processes in the individual level and one parameter at the population level. The three physiological processes are the feeding rate, length of the embryonic stage and respiration rate, and the population parameter is egg mortality.

Temperature is considered one of the most critical environmental factors affecting the success of fish (cf. [19, 62, 71, 80]). It has a direct effect on spawning, egg and larval development, activity, feeding, and, in general, on the growth of the fry and older life stages (i.e. after embryonic stage). Experimental studies have shown that increasing the temperature of the environment increases the respiratory metabolism and maintenance requirements of fish. In addition to the effects that excessively low and high temperature can have on fish, the level of dissolved oxygen also play an important role (cf. [13, 19, 20, 101]). The literature presents information and sources for a number of different species of fish which indicate how reduced levels of dissolved oxygen can have undesirable effects on physiological processes, including feeding, swimming ability, repiration, activity, fecundity and spawning activity. Experimental studies have shown that reduced levels of dissolved oxygen inhibit the developmental rate of the embryos and the time to hatching increases as well as the appearance of the various developmental stages. Also, other experimental studies that the size at hatching, the initial feeding, the percentage of larvae that suvive to the juvenile period, and, in general, the growth of embryos, are effected by the level of dissolved oxygen.

Although the numerical simulation code of this research do include the temperature and dissolved oxygen effects, the related numerical simulation examples are not included in this thesis. So, we here do not provide the details nor the mathematical formulations and functions of the temperature and dissolved oxygen effects on fish. For the details about theses mathematical formulations and functions, we refer to Lovelock [87] and the references therein.

1.4 Chemical Toxicant Effects

To study the impact of chemical stress on a biological system, Hallam *et al* [43, 44] state that in most cases this is best measured at the individual level, then extrapolated to the population and higher levels of biological organization. The degree of toxic chemical stress is related to level of chemical in a compartment of the body or in a target organ of the individual. The amount of chemical in the organism is determined by uptake from the biotic and abiotic environments. In our mathematical model, a toxicant uptake equation is applied to represent this procedure at individual level. Theoretically, there are lethal effects and sublethal effects which presents two different cases at population level. In real problems, these two effects usually occur simultaneously and combine together to influence the population dynamics. We discuss the combined effects in the numerical simulations in

Chemical Uptake Model in Individuals: To adequately address problems of ecotoxicology, it is necessary to consider the manner in which chemical exposure and the biological-chemical interfaces are formulated. The uptake of chemical from the environment and food represents the chemical exchange between the aqueous environment and the individual fish across the gill membranes and the chemical exchange between the fish and its intestinal food across the intestinal wall. The uptake model we use is a modification of FGETS developed by Barber *et al* (cf. [4]) to handle exposure of fish to non-polar, hydrophobic, reversible chemicals. The model was formulated based on the assumption that both environmental and food exposure are gradient-driven processes.

The mathematical model that describes the processes of chemical uptake from the environment and food and includes dilution of chemical due to organism growth is defined as:

$$\frac{dB_T}{da} = S_g k_w C_w + C_F F - \frac{B_T}{W_T\, BCF}(S_g k_w + E k_E) \tag{1.27}$$

where B_T represents the total toxicant in the organism; C_w and C_F represents the concentration of toxicant in the environment and in the food, respectively; F and E are the mass fluxes of food and feces, respectively; W_T is the total weight of the organism; BCF is the bioconcentration factor (total concentration in the organism$/C_w$); k_w is the unit conductance and k_E is the partition coefficient of chemical to excrement, which is given by $C_E\ /C_A$, where C_A and C_E are concentrations of the chemical toxicant in the aqueous portion of the organism and its feces, respectively. (1.27) is easy to handle numerically and mathematically since it looks linear in form. We are going to use this form of uptake equation to build our numerical scheme for individual-based fish population model with chemical toxicant effects. However, in order to understand the mechanism of toxicant effects easily, we need rewrite it as the following (1.28). Noting that $B_T = C_T \cdot W_T$, then we have, by plugging B_T into (1.27)

$$\frac{dC_T}{da} = k_1 C_w + \frac{F}{W_T} C_F - k_2 C_T - \frac{E k_E}{W_T} C_A - \frac{1}{V} \frac{dV}{da} C_T \tag{1.28}$$

where k_1 and k_2 are the uptake and deputation rates of the environmental chemical, respectively, and are specified by

$$\begin{aligned} k_1 &= S_g k_w V^{-1}, \\ k_2 &= S_g k_w V^{-1} (P_A + P_L K_L + P_S K_S)^{-1} \end{aligned}$$

and S_g is the exposed surface area. P_A, P_L, and P_S are the aqueous, lipid, and structural fractions of the organism, respectively; K_L is the partition coefficient of the chemical between the organism lipid and water; K_S is the partition coefficient of the chemical between the organism structure and water. Clearly, (1.28) stands for the dynamics of the total concentration of chemical toxicant in the whole fish, in particular, the last term of (1.28), $\frac{1}{V}\frac{dV}{da}C_T$, stands for the dilution of chemical toxicant due to organism growth.

Hypotheses imposed in the model development include the following. An individual organism is assumed to be comprised of three chemical phases: aqueous, structural, and lipid. The structural component is generally viewed as being composed of (physiologically active) protein and carbohydrates. A second hypothesis is that the time scales for the exchange across the exposed surface area, S_g, are regarded as being much slower than the distribution of chemical within the organism. Using this assumption, C_A is expressed in terms of C_T via

$$C_T = (P_A + P_L K_L + P_S K_S) C_A.$$

A third hypothesis was imposed to deal with difficulties of the transient events during digestive processes. The simplest assumption that avoids most of these difficulties is that of equilibration of chemical between the organism's body and the gut contents. This assumption, however, is not necessarily true. Hallam et al. [46] have indicated that this is the worst case assumption during increasing body concentration when exposed to contaminated food (i.e., no more chemical could be taken up under any thermodynamically consistent assumption than would be taken up when food and body equilibrate). During deputation, however, this assumption leads to predicted minimum deputation times; that is, any other thermodynamically consistent assumption would lead to longer predicted deputation times. For toxicity evaluations, this would usually not be considered the worst case scenario.

To calculate the concentration of the chemical in the food, we assume instantaneous chemical equilibration with the water and within the organism. The food, like the consumer, consists of the aqueous, lipid and structural phases and the chemical is distributed among them according to its affinity for these phases.

Lethal Effects: To model the effects of chemicals on individuals we need to couple the uptake model with models for the mode of action and models for concentration–response relations. Effects of chemicals on individuals focus on mortality but sublethal effects, such as reduction of growth rate, could be considered using a similar method [43, 58]. The assessment of mortality due to chemical action is implemented by utilizing formulations based upon quantitative structure–activity relations (QSARs). There are numerous QSARs in the literature for chemicals with different modes of action. We utilize results of Veith et al. [111] and Konemann [69] developed for baseline narcotic chemicals and relate a chemical property, the *octanol/water* partition coefficient, K_{ow}, to mortality of individuals (see Figure 1). For a single individual, an effect occurs when concentration of chemical in the aqueous phase reaches a critical level, denoted by LC_{50} (cf. Figure 4), and is calculated from the equation $\log LC_{50} = -0.8 - \log K_{ow}$.

The exposure–effect model is coupled with the physiologically–based individual model which yields expressions for the weight and surface area of the organism. This model of an individual fish includes lipid and structural components necessary for assessing effects of lipophilic chemicals on individuals. The aqueous component of an individual needed for the exposure model is assumed to be proportional to the structural mass of the individual.

Sublethal Effects: The chemical toxicant sublethal effects for fish have been discussed in [26], in which the same mechanism for the *Daphnia* is applied (cf. [43, 48]). While the toxicant effect is sublethal, the individual model (1.1) need to be modified since the chemical toxicant effects reduce the rate of accumulation of lipid and the rate of growth of structure at individual-level.

$$\begin{aligned} \frac{dm_L}{da} &= g_L \equiv \chi G_L - F_L \\ \frac{dm_S}{da} &= g_S \equiv \chi G_S - F_S \end{aligned} \tag{1.29}$$

where χ is the reduction in the accumulation and growth due to sublethal chemical effects. We choose the reduced rate of accumulation of lipid and the reduced rate of growth of structure for individual fish to be the same as ones for an individual

Daphnid as follows.

$$\chi = \begin{cases} 1 & \text{if } C_A < 10^{-1.83}K_{ow}^{-1} \\ 1 - \dfrac{1.37(C_A - 10^{-1.83}K_{ow}^{-1})}{0.0395K_{ow}^{-1} + C_A} & \text{if } 10^{-1.83}K_{ow}^{-1} \le C_A \le 10^{-0.8}K_{ow}^{-1} \\ 0 & \text{if } C_A > 10^{-0.8}K_{ow}^{-1} \end{cases} \tag{1.30}$$

where C_A is the internal aqueous concentration of chemical in an individual fish and K_{ow} is the *octanol/water* partition coefficient of the chemical. The value $10^{-1.83}K_{ow}^{-1}$ is the experimental no effect threshold. There is no effect on the growth of a fish, until C_A exceeds the threshold value $10^{-0.8}K_{ow}^{-1}$, the no growth threshold. While C_A exceeds this threshold, individual fish have a negative net growth rate, which only includes the loss functions.

Combined Effects: In our numerical simulations of Chapter 5, we consider the chemical toxicant effects combining the lethal and sublethal effects together. That is, the representation of chemical toxicant sublethal effects results in the growth reduction occurring continuously as a response to continuous internal toxicant concentration. Death of the organism caused by lethal toxicant effects is assumed to fall exactly at the time when the concentration in the aqueous phase of the fish reaches the value LC_{50} and, different from the growth, is quantally rather than continuously, assessed.

A summary of the related variables and parameters used in the uptake model is given in Table 3.

1.5 Individual-Based Population Models

In this section, we give a completed description of a mathematical model for individual-based fish populations in a spatially heterogeneous environment, which is studied in the rest of this thesis. The model consists of two parts: an individual model and population dynamic model. In particular, the population model here includes fish immigration in the older life stage (i.e. after the embryonic stage) due to diffusion and the environmental heterogeneity, for example, different concentrations of chemical toxicant and food density in the spatial domain (cf. [50, 83, 93, 96]). We here assume that fish live in a bounded connected spatial domain Ω with the flux type as in (1.11) or (1.12). We are going to use the same notations and definitions as previously given unless special declarations are presented.

We first consider the fish individual model. From Section 1.1, the fish individual model can be defined as follows:

Individual Model:

$$\begin{aligned}\frac{dm_L}{da} &\equiv g_L = G_L - F_L \\ \frac{dm_S}{da} &\equiv g_S = G_S - F_S\end{aligned} \tag{1.31}$$

$$\begin{aligned}m_L|_{a=0} &= m_{L_0} \\ m_S|_{a=0} &= m_{S_0}\end{aligned} \tag{1.32}$$

Furthermore, if the environment is polluted by a chemical toxicant and the toxicant effects on fish, then the fish individual model should be modified by including a chemical toxicant uptake equation and the toxicant effects on the fish growth. From Section 1.1 and 1.4, the fish individual model with toxicant effects can be written in the following.

Individual Model with Toxicant Effects:

$$\begin{aligned}\frac{dm_L}{da} &\equiv g_L = \chi G_L - F_L \\ \frac{dm_S}{da} &\equiv g_S = \chi G_S - F_S\end{aligned} \tag{1.33}$$

$$\begin{aligned}m_L|_{a=0} &= m_{L_0} \\ m_S|_{a=0} &= m_{S_0}\end{aligned} \tag{1.34}$$

$$\begin{aligned} \frac{dB_T}{da} &\equiv g_c = S_g k_w C_w + C_F F - \frac{B_T}{W_T BCF}(S_g k_w + E k_E) \\ B_T|_{a=0} &= B_{T_0} \end{aligned} \tag{1.35}$$

When the combined toxicant effects occurs, the growth rate of fish is reduced if the chemical concentration is less than the level LC_{50} by χ and fish is killed if the chemical concentration reaches the level LC_{50}.

We now consider population dynamic models. If fish might have movements due to both diffusion and advection as (1.11), the fish population dynamic model has been defined in Section 1.2, that is,

Population Dynamic Model (I):

$$\begin{gathered} \frac{\partial\rho}{\partial t} + \frac{\partial\rho}{\partial a} + \frac{\partial(\rho\, g_L)}{\partial m_L} + \frac{\partial(\rho\, g_S)}{\partial m_S} = -\mu\rho \\ \text{for } t \in (0,T], a \in (0,J], x \in \Omega, \end{gathered} \tag{1.36}$$

$$\begin{gathered} \frac{\partial\rho}{\partial t} + \frac{\partial\rho}{\partial a} + \frac{\partial(\rho\, g_L)}{\partial m_L} + \frac{\partial(\rho\, g_S)}{\partial m_S} - \nabla\cdot(k\nabla\rho - \mathbf{q}\cdot\rho) = -\mu\rho \\ \text{for } t \in (0,T], a \in (J,A_m], x \in \Omega, \end{gathered} \tag{1.37}$$

with the initial-boundary condition

$$\begin{aligned} & k(\frac{\partial\rho}{\partial\nu} - \mathbf{q}\cdot\nu) = 0 \quad \text{or} \quad \rho = 0, \quad x \in \partial\Omega\,, \\ & \rho(0,a,m_L,m_S,x) = \rho_0(a,m_L,m_S,x)\,, \\ & \rho(t,0,m_{0L},m_{0S},x) = \int_0^{A_m}\int_0^\infty\int_0^\infty \beta\rho(t,a,m_L,m_S,x)\,da\,dm_L\,dm_S \end{aligned} \tag{1.38}$$

By using the extensions (1.20) and (1.21), we can rewritten as a unified form:

Population Dynamics Model (I'):

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial a} + \frac{\partial(\rho\, g_L)}{\partial m_L} + \frac{\partial(\rho\, g_S)}{\partial m_S} - \nabla \cdot (\tilde{k}\, \nabla \rho - \mathbf{q} \cdot \rho) = -\mu\rho$$

$$\text{for } t \in (0,T], a \in [0, A_m], x \in \Omega, \tag{1.39}$$

$$\tilde{k}(\frac{\partial \rho}{\partial \nu} - \mathbf{q} \cdot \nu) = 0 \quad \text{or} \quad \rho = 0, \quad x \in \partial\Omega\,,$$

$$\rho(0, a, m_L, m_S, x) = \rho_0(a, m_L, m_S, x)\,, \tag{1.40}$$

$$\rho(t, 0, m_{0L}, m_{0S}, x) = \int_0^{A_m}\int_0^{\infty}\int_0^{\infty} \beta\rho(t, a, m_L, m_S, x)\, da\, dm_L\, dm_S$$

If fish have a pure diffusive movement as in (1.12), the fish population dynamic model is:

Population Dynamic Model (II):

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial a} + \frac{\partial(\rho\, g_L)}{\partial m_L} + \frac{\partial(\rho\, g_S)}{\partial m_S} = -\mu\rho \tag{1.41}$$

$$\text{for } t \in (0,T], a \in (0, J], x \in \Omega,$$

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial a} + \frac{\partial(\rho\, g_L)}{\partial m_L} + \frac{\partial(\rho\, g_S)}{\partial m_S} - \nabla \cdot (k \nabla \rho) = -\mu\rho \tag{1.42}$$

$$\text{for } t \in (0,T], a \in (J, A_m], x \in \Omega,$$

with the initial-boundary condition

$$
\begin{aligned}
&\tilde{k}\frac{\partial\rho}{\partial\nu} = 0 \quad \text{or} \qquad \rho = 0, \quad x \in \partial\Omega\,, \\
&\rho(0,a,m_L,m_S,x) = \ \rho_0(a,m_L,m_S,x)\,, \\
&\rho(t,0,m_{0L},m_{0S},x) = \ \int_0^{A_m}\int_0^{\infty}\int_0^{\infty}\beta\rho(t,a,m_L,m_S,x)\,da\,dm_L\,dm_S
\end{aligned}
\tag{1.43}
$$

Its unified form is:

Population Dynamics Model (II'):

$$
\begin{aligned}
&\frac{\partial\rho}{\partial t} + \frac{\partial\rho}{\partial a} + \frac{\partial(\rho\, g_L)}{\partial m_L} + \frac{\partial(\rho\, g_S)}{\partial m_S} - \nabla\cdot(\tilde{k}\,\nabla\rho) = \ -\mu\rho \\
&\qquad\qquad\qquad\qquad \text{for } t \in (0,T], a \in [0,A_m], x \in \Omega,
\end{aligned}
\tag{1.44}
$$

$$
\begin{aligned}
&\tilde{k}\frac{\partial\rho}{\partial\nu} = 0 \quad \text{or} \qquad \rho = 0, \quad x \in \partial\Omega\,, \\
&\rho(0,a,m_L,m_S,x) = \ \rho_0(a,m_L,m_S,x)\,, \\
&\rho(t,0,m_{0L`},m_{0S},x) = \ \int_0^{A_m}\int_0^{\infty}\int_0^{\infty}\beta\rho(t,a,m_L,m_S,x)\,da\,dm_L\,dm_S
\end{aligned}
\tag{1.45}
$$

Moreover, from the view point of biology and ecology, we assume that k, μ and β are nonnegative functions and dependent of the total population function $P = P(t,m_L,m_S,x)$. That is,

$$
\begin{aligned}
k &= \ k(t,x,P) \geq k_1 > 0 \\
\mu &= \mu(t,a,m_L,m_S,x,P) \geq 0 \\
\beta &= \ \beta(t,a,m_L,m_S,x,P) \geq 0
\end{aligned}
\tag{1.46}
$$

where

$$P = \int_0^{A_m} \rho(t, a, m_L, m_S, x)\, da. \tag{1.47}$$

We now can define the complete forms of individual-based population model, which are discussed in the rest of this thesis. We first consider that fish live in a heterogeneous spatial environment with diffusive and advective movements as in (1.11) at the older life stage (after embryonic stage). Then the individual-based population model can be defined as

$$\left.\begin{array}{l}\textbf{Individual Model} \;\; (1.31)\\ \textbf{Population Dynamic Model (I)} \;\; (1.41) - (1.42)\end{array}\right\} \tag{1.48}$$

or defined by using the unified form (1.22)

$$\left.\begin{array}{l}\textbf{Individual Model} \;\; (1.31)\\ \textbf{Population Dynamic Model(I}'\textbf{)} \;\; (1.39) - (1.43)\end{array}\right\} \tag{1.49}$$

Moreover, if there are chemical toxicant effects on fish, then the individual-based population model is

$$\left.\begin{array}{l}\textbf{Individual Model with Toxicant Effects} \;\; (1.33)\\ \textbf{Population Dynamic Model (I)} \;\; (1.41) - (1.42)\end{array}\right\} \tag{1.50}$$

or

$$\left.\begin{array}{l}\textbf{Individual Model with Toxicant Effects}\ \ (1.33)\\ \textbf{Population Dynamic Model (I}'\textbf{)}\ (1.39)-(1.43)\end{array}\right\}\tag{1.51}$$

As explained before, most of our analyses and discussions focus on the diffusion as in (1.12). Then, the above models with diffusion (1.12) can be rewritten as

$$\left.\begin{array}{l}\textbf{Individual Model}\ \ (1.31)\\ \textbf{Population Dynamic Model (II)}\ (3.110)--(3.111)\end{array}\right\}\tag{1.52}$$

or defined by using the unified form (1.24)

$$\left.\begin{array}{l}\textbf{Individual Model}\ \ (1.31)\\ \textbf{Population Dynamic Model (II}'\textbf{)}\ (1.44)-(3.112)\end{array}\right\}\tag{1.53}$$

Moreover, if there are chemical toxicant effects on fish, then

$$\left.\begin{array}{l}\textbf{Individual Model with Toxicant Effects}\ \ (1.33)\\ \textbf{Population Dynamic Model (II)}\ (1.41)-(1.42)\end{array}\right\}\tag{1.54}$$

or

$$\left.\begin{array}{l}\textbf{Individual Model with Toxicant Effects}\ \ (1.33)\\ \textbf{Population Dynamic Model (II}'\textbf{)}\ (1.44)-(3.112)\end{array}\right\}\tag{1.55}$$

It is not very hard to check that all of the above models are well-posed. Each of them is a mixed type problem of a ordinary differential system and a partial differential problem. In particular, the partial differential problem is a degenerate parabolic problem with discontinuous coefficients and nonlocal boundary conditions.

Chapter 2

Mathematical Models for Individual-Based Populations

In this chapter, we discuss mathematical models for individual-based, physiologically structured fish populations with diffusive and advective movement in a spatially heterogeneous environment defined in Section 1.5. The component models consist of representations of an individual fish and a fish population. From a biological point of view, the individual model depicts the growth of individual (or cohort) and the population dynamic model depicts the structural variation and distribution of the fish population. We have considered a fish population as well as the combined effects of chemical toxicant on a fish population in a spatially heterogeneous environment. From mathematical view point, our model is an initial problem for ordinary differential systems coupled with a nonlocal initial-boundary problem for nonlinear partial differential equations. The ordinary differential problem includes growth processes of the physiological variables and may also include a chemical toxicant uptake equation for chemical toxicant exposure which describes the various processes of chemical toxicant in a fish. The partial differential problem is a mixed problem of two coupled extended McKendrick-von Foerster type partial differential equations, which depicts fish population dynamics and distribution in two different age sets, the embryonic stage and older life stage. We consider fish in the time period $(0, T]$ and the age period $[0, A_m]$, where A_m is the maximum age. We also assume fish are in a connected spatial domain $\Omega \subset \mathcal{R}^{\mathbf{n}}$ $(\mathbf{n} = 1, 2, 3)$ with a smooth boundary $\partial\Omega$.

The individual-based, physiologically structured fish population mathematical models are presented. We then give a mathematical derivation for the mathematical models. Moreover, a primary mathematical analysis for the mathematical models is also shown, which contains the key idea to construct the computational models in Chapter 3. In addition, as a basis and preparation of mathematical analysis for the mathematical model, three closely related auxiliary age structured population dynamic models are discussed first. The first two have been studied before by several researchers (cf. [14, 37, 38, 77, 78, 79, 89]). The third is close to our model.

The notations in the previous chapter are utilized here. C represents a generic constant, which is only dependent the related given initial data and may take different values in the different places.

2.1 Mathematical Derivations

In this section, we show a mathematical derivation for the individual-based population mathematical models proposed in last section. Since the detailed mathematical derivations for the individual model, the chemical toxicant uptake equation, and the population dynamics without movements of Chapter 1 are already published (cf. [45, 47, 49, 46, 70, 89]), we here only give a mathematical derivation for the population dynamic model with spatial movements.

We consider a fish population, which is sufficiently dense so that a continuous theory can be applicable, and assume that the fish move in a bounded connected spatial region (open domain) $\Omega \subset \mathcal{R}^{\mathbf{n}}$ ($\mathbf{n} = 1, 2, 3$). Let $\rho(t, a, m_L, m_S, x)$ $(number/d \cdot g^2 \cdot m^{\mathrm{n}})$ be the density function, that is, the number of fish per age, per mass of lipid, per mass of structure, per volume of spatial environment at time t; where a represents age (d), $x \in \Omega$ represents the location.

Suppose that we arbitrarily choose the following variables such that

$$B \subset \Omega,\ \Delta t > 0,\ 0 < a_1 < a_2,\ 0 \le m_{L_1} < m_{L_2},\ 0 \le m_{S_1} < m_{S_2}.$$

Now we consider the variation of fish numbers in $B \times [a_1, a_2] \times [m_{L_1}, m_{L_2}] \times [m_{S_1}, m_{S_2}]$ from time t to time $t + \Delta t$, where when we say a fish is in B, that means, the fish is living in the spatial domain B; a fish in $[a_1, a_2]$, an age interval, means that the age of the fish is not greater than a_2 and is not less than a_1; similarly understanding applies for a fish in $[m_{L_1}, m_{L_2}]$ and $[m_{S_1}, m_{S_2}]$. Let $N(t)$ be the number of fish in $B \times [a_1, a_2] \times [m_{L_1}, m_{L_2}] \times [m_{S_1}, m_{S_2}]$ at time t, then,

$$N(t) = \int_B \int_{a_1}^{a_2} \int_{m_{L_1}}^{m_{L_2}} \int_{m_{S_1}}^{m_{S_2}} [\rho(t, a, m_L, m_S, x)]\, dx da dm_L dm_S.$$

Thus, the change of fish number in $B \times [a_1, a_2] \times [m_{L_1}, m_{L_2}] \times [m_{S_1}, m_{S_2}]$ from time t to time $t + \Delta t$ is:

$$\begin{aligned} N(t+\Delta t) - N(t) \;&=\; \int_B \int_{a_1}^{a_2} \int_{m_{L_1}}^{m_{L_2}} \int_{m_{S_1}}^{m_{S_2}} \\ &[\rho(t+\Delta t, a, m_L, m_S, x) - \rho(t, a, m_L, m_S, x)]\, dx da dm_L dm_S. \end{aligned} \tag{2.1}$$

On the other hand, we can calculate $N(t+\Delta t) - N(t)$ by counting how many fish come into $B \times [a_1, a_2] \times [m_{L_1}, m_{L_2}] \times [m_{S_1}, m_{S_2}]$ from outside in the time interval $[t,\ t + \Delta t]$, how many fish go out of $B \times [a_1, a_2] \times [m_{L_1}, m_{L_2}] \times [m_{S_1}, m_{S_2}]$ in the time interval $[t,\ t+\Delta t]$, and how many fish in $B \times [a_1, a_2] \times [m_{L_1}, m_{L_2}] \times [m_{S_1}, m_{S_2}]$ die in the time interval $[t,\ t + \Delta t]$. Then, $N(t + \Delta t) - N(t)$ can be expressed as

$$N(t + \Delta t) - N(t) = N_0 - N_1 - N_2 - N_3 + N_r, \tag{2.2}$$

where N_i $(i = 0, 1, 2, 3)$ and N_r will be defined. Let $\Delta m_L(t + \Delta t, a, m_L, m_S, \Delta t)$

and $\Delta m_S(t+\Delta t, a, m_L, m_S, \Delta t)$ be the average increase in the mass of lipid and structure of a fish of age a in the time interval $[t, t+\Delta t]$, respectively; and $\mathcal{D}$ be the flux through out of ∂B, the boundary of B.

N_0 represents the number of fish which are not in $[a_1, a_2] \times [m_{L_1}, m_{L_2}] \times [m_{S_1}, m_{S_2}]$ but are in B at time t, and which are in $B \times [a_1, a_2] \times [m_{L_1}, m_{L_2}] \times [m_{S_1}, m_{S_2}]$ at time $t+\Delta t$. The mathematical form of N_0 can be defined as follows

$$\begin{aligned} N_0 \;=\; & \int_B \int_{a_1-\Delta t}^{a_1} \int_{m_{L_1}-\Delta m_L(t+\Delta t, a+\Delta t, m_{L_1}, m_{S_1}, \Delta t)}^{m_{L_2}-\Delta m_L(t+\Delta t, a+\Delta t, m_{L_2}, m_{S_2}, \Delta t)} \int_{m_{S_1}-\Delta m_S(t+\Delta t, a+\Delta t, m_{L_1}, m_{S_1}, \Delta t)}^{m_{S_2}-\Delta m_S(t+\Delta t, a+\Delta t, m_{L_2}, m_{S_2}, \Delta t)} \\ & \quad [\rho(t, a, m_L, m_S, x)]\, dx\, da\, dm_L\, dm_S \\ & + \int_B \int_{a_1}^{a_2-\Delta t} \int_{m_{L_1}-\Delta m_L(t+\Delta t, a+\Delta t, m_{L_1}, m_{S_1}, \Delta t)}^{m_{L_2}-\Delta m_L(t+\Delta t, a+\Delta t, m_{L_2}, m_{S_2}, \Delta t)} \int_{m_{S_1}-\Delta m_S(t+\Delta t, a+\Delta t, m_{L_1}, m_{S_1}, \Delta t)}^{m_{S_1}} \\ & \quad [\rho(t, a, m_L, m_S, x)]\, dx\, da\, dm_L\, dm_S \\ & + \int_B \int_{a_1}^{a_2-\Delta t} \int_{m_{L_1}-\Delta m_L(t+\Delta t, a+\Delta t, m_{L_1}, m_{S_1}, \Delta t)}^{m_{L_1}} \int_{m_{S_1}}^{m_{S_2}-\Delta m_S(t+\Delta t, a+\Delta t, m_{L_2}, m_{S_2}, \Delta t)} \\ & \quad [\rho(t, a, m_L, m_S, x)]\, dx\, da\, dm_L\, dm_S. \end{aligned}$$

N_1 represents the number of fish which are in $B \times [a_1, a_2] \times [m_{L_1}, m_{L_2}] \times [m_{S_1}, m_{S_2}]$ at time t, but are not in $[a_1, a_2] \times [m_{L_1}, m_{L_2}] \times [m_{S_1}, m_{S_2}]$ and are still in B at time $t + \Delta t$. The mathematical form of N_1 is defined as

$$\begin{aligned}
N_1 &= \int_B \int_{a_2-\Delta t}^{a_2} \int_{m_{L_1}}^{m_{L_2}} \int_{m_{S_1}}^{m_{S_2}} [\rho(t, a, m_L, m_S, x)]\, dx da dm_L dm_S \\
&\quad + \int_B \int_{a_1}^{a_2-\Delta t} \int_{m_{L_1}}^{m_{L_2}} \int_{m_{S_2}-\Delta m_S(t+\Delta t, a+\Delta t, m_{L_2}, m_{S_2}, \Delta t)}^{m_{S_2}} \\
&\qquad [\rho(t, a, m_L, m_S, x)]\, dx da dm_L dm_S \\
&\quad + \int_B \int_{a_1}^{a_2-\Delta t} \int_{m_{L_2}-\Delta m_L(t+\Delta t, a+\Delta t, m_{L_2}, m_{S_2}, \Delta t)}^{m_{L_2}} \int_{m_{S_1}}^{m_{S_2}-\Delta m_S(t+\Delta t, a+\Delta t, m_{L_2}, m_{S_2}, \Delta t)} \\
&\qquad [\rho(t, a, m_L, m_S, x)]\, dx da dm_L dm_S.
\end{aligned}$$

N_2 represents the number of fish which are not in B at time t, but are in $B \times [a_1, a_2] \times [m_{L_1}, m_{L_2}] \times [m_{S_1}, m_{S_2}]$ at time $t + \Delta t$. N_2 is defined as

$$\begin{aligned}
N_2 &= \int_t^{t+\Delta t} \int_{a_1-\Delta t+\tau}^{a_2-\Delta t+\tau} \int_{m_{L_1}-\Delta m_L(t+\Delta t, a+\Delta t, m_{L_1}, m_{S_1}, t+\Delta t)-\tau}^{m_{L_1}-\Delta m_L(t+\Delta t, a+\Delta t, m_{L_2}, m_{S_2}, t+\Delta t)-\tau} \\
&\quad \int_{m_{S_1}-\Delta m_S(t+\Delta t, a+\Delta t, m_{L_1}, m_{S_1}, t+\Delta t)-\tau}^{m_{S_2}-\Delta m_S(t+\Delta t, a+\Delta t, m_{L_2}, m_{S_2}, t+\Delta t)-\tau} \left(\int_{\partial B} \mathcal{D} \cdot \nu ds \right) d\tau da dm_L dm_S.
\end{aligned}$$

where ν is the outer unit normal direction of ∂B.

N_3 represents the number of fish which were in $B \times [a_1, a_2] \times [m_{L_1}, m_{L_2}] \times [m_{S_1}, m_{S_2}]$ in the time interval $[t,\ \Delta t]$ and who died in time interval $[t, t + \Delta t]$.

This is defined in the following

$$\begin{aligned}
N_3 &= \int_B \int_t^{t+\Delta t} \int_{a_1-\Delta t+\tau}^{a_2-\Delta t+\tau} \int_{m_{L_1}-\Delta m_L(t+\Delta t,a+\Delta t,m_{L_1},m_{S_1},t+\Delta t)-\tau}^{m_{L_1}-\Delta m_L(t+\Delta t,a+\Delta t,m_{L_2},m_{S_2},t+\Delta t)-\tau} \\
&\quad \int_{m_{S_1}-\Delta m_S(t+\Delta t,a+\Delta t,m_{L_1},m_{S_1},t+\Delta t)-\tau}^{m_{S_2}-\Delta m_S(t+\Delta t,a+\Delta t,m_{L_2},m_{S_2},t+\Delta t)-\tau} \\
&\quad [\mu\rho(t,a,m_L,m_S,x)]dxd\tau dadm_Ldm_S.
\end{aligned}$$

N_r represents the portion of N_3 which also belong to N_2. So, it has been calculated twice, once in N_2 and once in N_3. This can be estimated as

$$\begin{aligned}
N_r &\leq \Bigg| \int_t^{t+\Delta t} \mu \int_t^{\tau} \int_{a_1-\Delta t+\tau}^{a_2-\Delta t+\tau} \int_{m_{L_1}-\Delta m_L(t+\Delta t,a+\Delta t,m_{L_1},m_{S_1},t+\Delta t)-\tau}^{m_{L_1}-\Delta m_L(t+\Delta t,a+\Delta t,m_{L_2},m_{S_2},t+\Delta t)-\tau} \\
&\quad \int_{m_{S_1}-\Delta m_S(t+\Delta t,a+\Delta t,m_{L_1},m_{S_1},t+\Delta t)-\tau}^{m_{S_2}-\Delta m_S(t+\Delta t,a+\Delta t,m_{L_2},m_{S_2},t+\Delta t)-\tau} (\int_{\partial B} \mathcal{D}\cdot \nu ds) dt d\tau dadm_Ldm_S \Bigg| \\
&= O((\Delta t)^2).
\end{aligned}$$

Hence, using the Mean Value Theorem for Integration, Mean Value Theorem for Differentiation, Gauss Divergence Theorem (cf. [34, 117]) and individual model (2.51), we have that by direct computation

$$\begin{aligned}
\lim_{\Delta t\to 0} \frac{N_0}{\Delta t} &= \int_B \int_{m_{L_1}}^{m_{L_2}} \int_{m_{S_1}}^{m_{S_2}} \rho(t,a_1,m_L,m_S,x)dxdm_Ldm_S \\
&\quad + \int_B \int_{a_1}^{a_2} \int_{m_{L_1}}^{m_{L_2}} \left[(g_S|_{(m_{L_1},m_{S_1})})\rho(t,a,m_L,m_{S_1},x)\right] dxdadm_L
\end{aligned}$$

$$+\int_B \int_{a_1}^{a_2} \int_{m_{S_1}}^{m_{S_2}} \left[(g_L|_{(m_{L_1},m_{S_1})})\rho(t,a,m_{L_1},m_S,x)\right] dxdadm_S.$$

$$\begin{aligned}
\lim_{\Delta t\to 0}\frac{N_1}{\Delta t} &= \int_B \int_{m_{L_1}}^{m_{L_2}} \int_{m_{S_1}}^{m_{S_2}} \rho(t,a_2,m_L,m_S,x)dxdm_Ldm_S \\
&\quad +\int_B \int_{a_1}^{a_2} \int_{m_{L_1}}^{m_{L_2}} \left[(g_S|_{(m_{L_2},m_{S_2})})\rho(t,a,m_L,m_{S_2},x)\right] dxdadm_L \\
&\quad +\int_B \int_{a_1}^{a_2} \int_{m_{S_1}}^{m_{S_2}} \left[(g_L|_{(m_{L_2},m_{S_2})})\rho(t,a,m_{L_2},m_S,x)\right] dxdadm_S.
\end{aligned}$$

$$\lim_{\Delta t\to 0}\frac{N_2}{\Delta t} = \int_B \int_{a_1}^{a_2} \int_{m_{L_1}}^{m_{L_2}} \int_{m_{S_1}}^{m_{S_2}} (\nabla\cdot\mathcal{D})dxdadm_Ldm_S.$$

$$\lim_{\Delta t\to 0}\frac{N_3}{\Delta t} = \int_B \int_{a_1}^{a_2} \int_{m_{L_1}}^{m_{L_2}} \int_{m_{S_1}}^{m_{S_2}} \left[\mu\rho(t,a,m_L,m_S,x)\right] dxdadm_Ldm_S.$$

Then, the above four formulas, together with (2.2) and the basic theorem for calculus, imply that

$$\begin{aligned}
&\lim_{\Delta t\to 0}\frac{N(t+\Delta t)-N(t)}{\Delta t} \\
&= -\int_B \int_{a_1}^{a_2} \int_{m_{L_1}}^{m_{L_2}} \int_{m_{S_1}}^{m_{S_2}} \left[\frac{\partial\rho}{\partial a}+\frac{\partial(g_L\rho)}{\partial m_L}+\frac{\partial(g_S\rho)}{\partial m_S}\right] dxdadm_Ldm_S
\end{aligned}$$

$$+\int_B \int_{a_1}^{a_2} \int_{m_{L_1}}^{m_{L_2}} \int_{m_{S_1}}^{m_{S_2}} [\nabla\mathcal{D} - \mu\rho(t,a,m_L,m_S,x)]\, dx da dm_L dm_S.$$

On the other hand, it follows from (2.1) that

$$\lim_{\Delta t\to 0} \frac{N(t+\Delta t) - N(t)}{\Delta t} = \int_B \int_{a_1}^{a_2} \int_{m_{L_1}}^{m_{L_2}} \int_{m_{S_1}}^{m_{S_2}} \frac{\partial \rho}{\partial t} dx da dm_L dm_S.$$

Therefore, we obtain that

$$\begin{aligned}
&\int_B \int_{a_1}^{a_2} \int_{m_{L_1}}^{m_{L_2}} \int_{m_{S_1}}^{m_{S_2}} \frac{\partial \rho}{\partial t} dx da dm_L dm_S \\
&= -\int_B \int_{a_1}^{a_2} \int_{m_{L_1}}^{m_{L_2}} \int_{m_{S_1}}^{m_{S_2}} \left[\frac{\partial \rho}{\partial a} + \frac{\partial (g_L\rho)}{\partial m_L} + \frac{\partial (g_S\rho)}{\partial m_S}\right] dx da dm_L dm_S \qquad (2.3) \\
&+ \int_B \int_{a_1}^{a_2} \int_{m_{L_1}}^{m_{L_2}} \int_{m_{S_1}}^{m_{S_2}} [\nabla\cdot\mathcal{D} - \mu\rho(t,a,m_L,m_S,x)]\, dx da dm_L dm_S.
\end{aligned}$$

In view of the arbitrary character of B, a_1, $a_2, \cdots$, (2.3) immediately implies

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial a} + \frac{\partial (g_L\rho)}{\partial m_L} + \frac{\partial (g_S\rho)}{\partial m_S} - \nabla\cdot\mathcal{D} = -\mu\rho. \qquad (2.4)$$

If we consider a non-spatial model, or one without fish movement, we can simply take $\mathcal{D} = 0$. Hence, (2.4) implies the nonspatial (or without any movements) population dynamic model (cf. [89]) (where we may just regard x as a parameter not a variable for the differential equation). In general, there are many types of fish movements. We now list some typical cases as follows.

Case 1. If we consider the advection movement case so that fish alter their movement in response to conspecifics and/or environment spatial heterogeneity, then we take $\mathcal{D} = \rho\, \mathbf{q}(t, a, m_L, m_S, x, P)$. Hence, (2.4) implies that (cf. [50, 83, 96])

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial a} + \frac{\partial (g_L \rho)}{\partial m_L} + \frac{\partial (g_S \rho)}{\partial m_S} + \nabla \cdot (\rho \mathbf{q}) = -\mu \rho.$$

Case 2. If we consider the directed dispersal in the direction of least crowding, then we take $\mathcal{D} = k\, \rho\, \nabla P$. Hence, (2.4) implies that (cf. [11, 91, 96])

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial a} + \frac{\partial (g_L \rho)}{\partial m_L} + \frac{\partial (g_S \rho)}{\partial m_S} - \nabla \cdot (k\, \rho \nabla P) = -\mu \rho.$$

Case 3. If we treat random dispersal so that the local flow of population lies in the direction of decreasing density, then we take $\mathcal{D} = k\, \nabla\, \rho$. Hence, (2.4) is just the model (1.10) with $\mathcal{D}$ as in (1.12), that is, the individual-based model for fish population dynamics with diffusion (cf. [17, 96]).

Case 4. When we assume that fish do not make any spatial movement in the embryonic stage $(0, J]$ but do have movements in the older life stage $(J, A_m]$, then we should choose that $\mathcal{D} = \tilde{k}\, \nabla\, \rho$ where $\tilde{k}$ is defined as in (1.20). Hence, we obtain the model (1.24).

Case 5. We may mix some of the above cases, in particular, diffusion and convection. For example, $\mathcal{D} = k\, \nabla\, \rho - \mathbf{q}\, \rho$, then the population model is (1.10) with $\mathcal{D}$

as in (1.11), and $\mathcal{D} = \tilde{k} \nabla \rho - \tilde{\mathrm{q}} \rho$, then the population model is (1.22).

2.2 Age Structured Population Dynamic Problems

In order to give a mathematical analysis for the mathematical model for individual-based fish populations proposed in the previous sections, we first consider three auxiliary age structured population dynamic models as preparations to understand more complex models, for instance, our model. In particular, we are going to show some results about the existence, uniqueness and properties for the solutions.

We now discuss the first auxiliary age structured population dynamic model defined as follows, which has been discussed in [38, 89, 93, 115, 114].

Age Structured Population Problem (I)

$$\begin{aligned} \frac{\partial u}{\partial t} + \frac{\partial u}{\partial a} &= -\mu u \\ u(0,a) &= u_0(a) \\ u(t,0) &= \int_0^{A_m} \beta u(t,a)\, da \end{aligned} \tag{2.5}$$

where $\mu = \mu(t,a,P)$, $\beta = \beta(t,a,P)$, and

$$P \equiv P(t) = \int_0^{A_m} u(t,a)\, da,$$

and where A_m is the maximum age; this means we assume that

$$u(t, A_m) = 0, \qquad \forall t \in (0, T]$$

By the method of characteristics, we have (cf. [89, 114])

LEMMA 1 *Assume that* μ *is a nonnegative continuous function over* $[0,T] \times [0, A_m)$ *and* β *is a nonnegative bounded continuous function over* $[0,T] \times [0, A_m]$. *There then exists a unique classic solution of* (2.5) *satisfying*

$$0 \leq u(t,a) \leq C, \qquad \forall t \in (0,T], \quad a \in [0, A_m]$$

where C *is a constant, only dependent on the given initial data.*

The second auxiliary age structured population dynamic model is an age structured model with diffusion and defined as follows, which has been studied in [7, 29, 38, 41, 42, 77, 78, 79, 115].

Age Structured Population Problem (II)

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial a} - \nabla \cdot (k \nabla u) = -\mu u \tag{2.6}$$

$$
\begin{aligned}
&k\frac{\partial u}{\partial \nu} = 0 \quad or \quad u = 0, \quad \text{on} \quad \partial\Omega \\
&u(0,a,x) = u_0(a,x) \qquad\qquad (2.7) \\
&u(t,0,x) = B(t,x)
\end{aligned}
$$

where $k = k(t,x,P)$, $\mu = \mu(t,a,x,P)$, and

$$
P \equiv P(t,x) = \int_0^{A_m} u(t,a,x)da.
$$

We first consider that $B(t,x)$ is a given function and then $B(t,x)$ is defined by the renewal equation. Clearly, the weak formulation of problem (2.6)–(2.7) is: Find $u : (0,T] \times [0,A_m] \longrightarrow V$ such that

$$
\begin{aligned}
&(\partial_\tau u, w) + \alpha(k,u,w) = -(\mu u, w), \quad \text{for } \forall\ w \in V \\
&u(0,a,x) = u_0(a,x) \qquad\qquad (2.8) \\
&u(t,0,x) = B(t,x)
\end{aligned}
$$

where $(\cdot,\ \cdot)$ is the inner product of $L^2(\Omega)$, and

$$
\partial_\tau u = \frac{\partial u}{\partial t} + \frac{\partial u}{\partial a} \qquad (2.9)
$$

$$
\alpha(k,v,w) = (k\nabla u, \nabla w) = \int_\Omega k\nabla u\nabla w dx \qquad (2.10)
$$

$$V = \begin{cases} H^1(\Omega), & \text{when} \quad k\,\dfrac{\partial u}{\partial \nu} = 0 \\ H_0^1(\Omega), & \text{when} \quad u = 0. \end{cases} \tag{2.11}$$

Here and later on, $H^m(\Omega)$ ($H_0^m(\Omega)$) and $W^{m,q}(\Omega)$ ($W_0^{m,q}(\Omega)$) are the standard Sobolev spaces (cf. [1, 34, 63]), whose standard norms (semi-norms) are denoted as $\|\cdot\|_m$ ($|\cdot|_m$) and $\|\cdot\|_{m,q}$ ($|\cdot|_{m,q}$), respectively. By semigroup theory, linearization and delay techniques (cf. [89, 78, 115, 114, 117]), we then have the following lemmas (cf. [77, 78, 79, 115]).

LEMMA 2 *Assume that μ is a nonnegative continuous function and has bounded first derivatives with respect to all of its variables. Also assume that k is a positive continuous function and has a bounded first derivative $\frac{\partial k}{\partial P}$, more precisely,*

$$k_2 \geq k \geq k_1 > 0, \quad |\frac{\partial k}{\partial P}| \leq C_k$$

where k_1, k_2 and C_k are constants. Let $B(t,x) \in L^2((0,T],\ V)$ $u_0(a,x) \in L^2([0,A_m],\ V)$ be given. Then there exists a nonnegative solution of (2.8). *Moreover, we have that*

(i) if both k and μ are independent of P, the solution of (2.8) *is unique.*

(ii) if k is independent of P, $B(t,x) \in L^2((0,T],\ V \cap L^\infty(\Omega))$, and $u_0(a,x) \in L^2([0,A_m],\ V \cap L^\infty(\Omega))$, there exists a unique solution of (2.8) *$u \in L^2((0,T] \times 0, A_m],\ V \cap L^\infty(\Omega))$.*

(iii) if $B(t,x) \in L^2((0,T],\ V \cap W^{1,\infty}(\Omega))$, and $u_0(a,x) \in L^2([0,A_m],\ V \cap$

$W^{1,\infty}(\Omega)$), there exists a unique solution of (2.8) $u \in L^2((0,T] \times [0,A_m], V \cap W^{1,\infty}(\Omega))$.

We are ready to consider the other case for which $B(t,x)$ is replaced by the renewal equation, i.e.,

$$B(t,x) = \int_0^{A_m} \beta u(t,a,x) da$$

where $\beta = \beta(t,a,x,P)$ is the birth rate. Therefore, we can rewrite the problem as follows

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial a} - \nabla \cdot (k \nabla u) = -\mu u \tag{2.12}$$

$$\begin{aligned} & k\frac{\partial u}{\partial \nu} = 0 \quad \textit{or} \quad u = 0, \quad \text{on} \quad \partial\Omega \\ & u(0,a,x) = u_0(a,x) \\ & u(t,0,x) = \int_0^{A_m} \beta u(t,a,x) da. \end{aligned} \tag{2.13}$$

Its weak formulation is: Find $u : (0,T] \times [0,A_m] \longrightarrow V$ such that

$$\begin{aligned} & (\partial_\tau u,\ w) + \alpha(k,u,w) = -(\mu u, w), \quad \text{for } \forall\ w \in V \\ & u(0,a,x) = u_0(a,x) \\ & u(t,0,x) = \int_0^{A_m} \beta u(t,a,x) da. \end{aligned} \tag{2.14}$$

We also can have a similar lemma as Lemma 2 (cf. [73, 77, 78, 79, 114]).

LEMMA 3 *Assume that μ is a nonnegative continuous function and has bounded* *first derivatives with respect to all of its variables. Also assume that* k *and* β *are nonnegative continuous functions and have a bounded first derivative with respect to* P*, that is,*

$$\begin{aligned} &k_2 \geq k \geq k_1 > 0, \quad |\frac{\partial k}{\partial P}| \leq C_k \\ &\bar{\beta} \geq \beta \geq 0, \quad |\frac{\partial \beta}{\partial P}| \leq C_\beta \end{aligned}$$

where k_1, k_2 , $\bar{\beta}$, C_k *and* C_β *are constants. Let* $u_0(a,x) \in L^2([0,A_m],\ V)$ *be given. Then there exists a nonnegative solution of* (2.14)*. Moreover,*

(i) if both k, μ *and* β *are independent of* P*, the solution of* (2.14) *is unique.*

(ii) if k *is independent of* P *and* $u_0(a,x) \in L^2([0,A_m],\ V \cap L^\infty(\Omega))$*, there exists a unique solution of* (2.14) $u \in L^2((0,T] \times 0, A_m],\ V \cap L^\infty(\Omega))$.

(iii) if $u_0(a,x) \in L^2([0,A_m],\ V \cap W^{1,\infty}(\Omega))$ *, there exists a unique solution of* (2.14) $u \in L^2((0,T] \times 0, A_m],\ V \cap W^{1,\infty}(\Omega))$.

Furthermore, from the analyses and proofs for Lemma 2 and Lemma 3 in [89, 78, 115, 114], it is not hard to see that Lemma 2 and Lemma 3 can be extended to the model with both diffusion and advection (see **Remark 2.3.1**).

Finally, we consider the third auxiliary age structured population dynamic model, which is a mixed type model that combines the above two auxiliary age structured population dynamic models. In the model, we assume that fish do not move in the embryonic stage and may move only during the older life stage (after the embryonic stage). This is a reasonable assumption in biology. However, from a mathematical perspective, this brings some new difficulties since the partial differential equation now is a mixed type equation with discontinuous coefficients.

Mixed Age Structured Population Problem (III)

$$\begin{aligned} &\frac{\partial u}{\partial t} + \frac{\partial u}{\partial a} = -\mu\, u \\ &\qquad\qquad \text{for } t \in (0,T], a \in (0,J], x \in \Omega \end{aligned} \tag{2.15}$$

$$\begin{aligned} &\frac{\partial u}{\partial t} + \frac{\partial u}{\partial a} + \nabla \cdot (k \nabla\, u) = -\mu\, u \\ &\qquad\qquad \text{for } t \in (0,T], a \in (J,A], x \in \Omega \end{aligned} \tag{2.16}$$

$$\begin{aligned} &k\frac{\partial u}{\partial \nu} = 0 \quad \text{or} \quad u = 0, \quad \text{on} \quad \partial\Omega \\ &u(0,a,x) = u_0(a,x) \\ &u(t,0,x) = B(t,\, x) \end{aligned} \tag{2.17}$$

where μ, k, B and P have the same definitions and assumptions as those in the above auxiliary age structured problem (II). If we extend k to $\tilde{k}$ as in (1.20), we can combine (3.82) and (3.83) as the unified form:

$$\begin{aligned} &\frac{\partial u}{\partial t} + \frac{\partial u}{\partial a} - \nabla \cdot (\tilde{k}\, \nabla u) = -\mu\, u \\ &\qquad\qquad \text{for } \forall\ t \in [0,T], a \in [0,A_m], x \in \Omega. \end{aligned} \tag{2.18}$$

Its corresponding weak form is: Find $u : (0,T] \times [0, A_m] \longrightarrow V$, such that

$$
\begin{aligned}
&(\partial_\tau u,\ w) + \alpha(\tilde{k},\ u,\ w) = -(\mu u,\ w), \quad \text{for } \forall\ w \in V \\
&u(0,a,x) = u_0(a,\ x) \qquad\qquad\qquad\qquad\qquad\qquad (2.19) \\
&u(t,0,x) = \ B(t,\ x).
\end{aligned}
$$

LEMMA 4 *Assume that μ is a nonnegative continuous function and has bounded first derivatives with respect to all of its variables. Also assume that k is a positive continuous function and has a bounded first derivative $\frac{\partial k}{\partial P}$, more precisely,*

$$
k_2 \geq k \geq k_1 > 0, \quad |\frac{\partial k}{\partial P}| \leq C_k
$$

where k_1, k_2 and C_k are constants. Let $B(t,x) \in L^2((0,T],\ V)$ and $u_0(a,x) \in L^2([0,A_m],\ V)$ be given. Then

(i) if both k and μ are independent of P, there exists at most one weak solution of (2.19).

(ii) if k is independent of P, $B(t,x) \in L^2((0,T],\ V \cap L^\infty(\Omega)\,)$, and $u_0(a,x) \in L^2([0,A_m],\ V \cap L^\infty(\Omega))$, there exists at most one solution of (2.19) *$u \in L^2((0,T] \times [0,A_m],\ V \cap L^\infty(\Omega)\,)$.*

(iii) if $B(t,x) \in L^2((0,T],\ V \cap W^{1,\infty}(\Omega)\,)$ and $u_0(a,x) \in L^2([0,A_m],\ V \cap W^{1,\infty}(\Omega)\,)$, there exists at most one solution of (2.19) *$u \in L^2((0,T] \times [0,A_m],\ V \cap W^{1,\infty}(\Omega)\,)$.*

Proof. We here only discuss *(iii)* since a small modification and simplification of this proof implies immediately *(i)* and *(ii)*. Let $u_1,\ u_2\ \in\ L^2([0,A_m],\ V\cap W^{1,\infty}(\Omega)\ )$ be two weak solutions of (2.19). Then, there is a constant $M > 0$, such that

$$\int_0^T \int_0^{A_m} \|u_i\|_{1,\infty}\, dt\, da \ \le\ M^2, \qquad (i = 1,\ 2). \tag{2.20}$$

Moreover, denote by

$$\begin{aligned} &v_i \ =\ \exp(-\lambda\, t)\, u_i, \quad P_i = \int_0^{A_m} u_i\, da, \quad (i = 1,\ 2) \\ &\tilde{k}^*(P) = \tilde{k}(t,a,x,P), \quad \mu^*(P) = \mu(t,a,x,P) \\ &w \ =\ v_1\ -\ v_2 \end{aligned} \tag{2.21}$$

where λ is a positive constant, which will be determined later. Hence, it follows from (2.19) that, for w and v_i $(i = 1,2)$,

$$w(0,a,x) \ =\ w(t,0,x) \ =\ 0, \quad \text{for } \ x \in \Omega$$

$$(\partial_\tau\, v_i,\ w) + \alpha(\tilde{k}^*(P_i),\ u,\ w) + (\ (\mu^*(p_i) + \lambda)\, v_i,\ w) = 0. \tag{2.22}$$

By elementary computations, we have that

$$\int_0^T \int_0^{A_m} \Big[\alpha(\tilde{k}^*(P_1),\ v_1,\ w) - \alpha(\tilde{k}^*(P_2),\ v_2,\ w)\Big]\, dt\, da$$

$$= \int_0^T \int_J^{A_m} \left[\alpha(\tilde{k}^*(P_1),\, v_1,\, w) - \alpha(\tilde{k}^*(P_2),\, v_2,\, w)\right] dt\, da$$

$$= \int_0^T \int_J^{A_m} \left[(\tilde{k}^*(P_1)\nabla w,\ \nabla w) + ((\tilde{k}^*(P_1) - \tilde{k}^*(P_2))\, \nabla v_2,\ \nabla w)\right] dt\, da$$

$$\geq\ k_1 \int_0^T \int_J^{A_m} |w|_1^2\, dt\, da - C\int_0^T \int_J^{A_m} |((P_1 - P_2)\, \nabla v_2,\ \nabla w)|\, dt\, da$$

$$= \ k_1 \int_0^T \int_J^{A_m} |w|_1^2\, dt\, da$$
$$-C\int_0^T \int_J^{A_m} \left| \int_\Omega \left(\int_0^{A_m} (v_1 - v_2)\, da \right) \nabla u_2 \cdot \nabla w dx \right| dt\, da$$

$$\geq\ k_1 \int_0^T \int_J^{A_m} |w|_1^2\, dt\, da$$
$$-CM \left[\int_0^T \int_J^{A_m} \left(\int_\Omega \left| \int_0^{A_m} w\, da \right| \cdot |\nabla w|\, dx \right)^2 dt\, da \right]^{1/2}$$

$$\geq\ k_1 \int_0^T \int_J^{A_m} |w|_1^2\, dt\, da$$
$$-CM \left[\int_0^T \int_J^{A_m} \left(\int_\Omega \int_0^{A_m} |w|^2\ dx\, da \int_\Omega |\nabla w|^2 dx \right)\ dt\, da \right]^{1/2}$$

$$\geq\ k_1 \int_0^T \int_J^{A_m} |w|_1^2\, dt\, da - \int_0^T \int_J^{A_m} \left[CM \int_0^{A_m} \|w\|_0^2 da + \frac{k_1}{2}\, |w|_1^2 \right] dt\, da$$

$$\geq\ -CM \int_0^T \int_0^{A_m} \|w\|_0^2\, dt\, da \tag{2.23}$$

and we have that

$$\int_0^T \int_0^{A_m} [\,(\mu^*(P_1)\,v_1,\ w) - (\mu^*(P_2)\,v_1,\ w)\,]\,dt\,da$$

$$= \int_0^T \int_0^{A_m} [\,(\mu^*(P_1)\,w,\ w) + ((\mu^*(P_1) - \mu^*(P_2))\,v_2,\ w)\,]\,dt\,da$$

$$\geq\ -C\int_0^T \int_0^{A_m} |((P_1 - P_2)\,v_2,\ w)|\ dt\,da$$

$$=\ -C\int_0^T \int_0^{A_m} \left| \int_\Omega \left(\int_0^{A_m} (v_1 - v_2)\,da \right)\ u_2\,w dx \right|\ dt\,da$$

$$\geq\ -CM\left[\int_0^T \int_0^{A_m} \left(\int_\Omega \left| \int_0^{A_m} w da \right| \cdot |w|\ dx \right)^2\ dt\,da \right]^{1/2}$$

$$\geq\ -CM\left[\int_0^T \int_0^{A_m} \left(\int_0^{A_m} \int_\Omega |w|^2\,dx\,da \int_\Omega |w|^2\,dx \right)\ dt\,da \right]^{1/2}$$

$$\geq\ -CM\int_0^T \int_0^{A_m} \left[\int_0^{A_m} \|w\|_0^2 da + \|w\|_0^2 \right] dt\,da$$

$$\geq\ -CM\int_0^T \int_0^{A_m} \|w\|_0^2\,dt\,da. \tag{2.24}$$

Therefore, integrating (2.22) over $[0,\ T] \times [0, A_m]$ and taking the difference of the two equalities $(i = 1, 2)$, we have that

$$\begin{aligned}
0 &= \int_0^T \int_0^{A_m} [(\partial_\tau w,\, w) + \lambda(w,\, w) + (\,\alpha(\tilde{k}^*(P_1),\, v_1,\, w) - \alpha(\tilde{k}^*(P_2),\, v_2,\, w)\,) \\
&\qquad +(\,(\mu^*(P_1)\, v_1,\; w) - (\mu^*(P_2)\, v_1,\; w)\,)]dt\, da \\
&\geq \frac{1}{2}\int_0^T \int_0^{A_m} \left[\frac{\partial(\|w\|_0^2)}{\partial t} + \frac{\partial(\|w\|_0^2)}{\partial a}\right] dt\, da \\
&\qquad +\lambda \int_0^T \int_0^{A_m} \|w\|_0^2\, dt\, da - CM \int_0^T \int_0^{A_m} \|w\|_0^2\, dt\, da \\
&= \frac{1}{2}\left[\int_0^T \|w(t, A_m, \cdot)\|_0^2\, dt + \int_0^{A_m} \|w(T, a, , \cdot)\|_0^2\, da\right] \\
&\qquad +\lambda \int_0^T \int_0^{A_m} \|w\|_0^2\, dt\, da - CM \int_0^T \int_0^{A_m} \|w\|_0^2\, dt\, da \\
&\geq (\lambda - CM\,) \int_0^T \int_0^{A_m} \|w\|_0^2\, dt\, da.
\end{aligned}$$

Thus, by taking λ large enough, this implies that

$$\int_0^T \int_0^{A_m} \|w\|_0^2\, dt\, da \leq 0.$$

Clearly, that means that $w = v_1 - v_2 = 0$. Hence, $u_1 = u_2$. So we have proved this Lemma.

THEOREM 1 *With the same assumptions as Lemma 4, then we have that* *(i) if both k and μ are independent of P, there exists a unique weak solution of* (2.19).

(ii) if k is independent of P, $B(t,x) \in L^2((0,T],\ V \cap L^\infty(\Omega))$, and $u_0(a,x) \in L^2([0,A_m],\ V \cap L^\infty(\Omega))$, there exists a unique solution of (2.19) $u \in L^2((0,T] \times [0,A_m],\ V \cap L^\infty(\Omega))$.

(iii) if $B(t,x) \in L^2((0,T],\ V \cap W^{1,\infty}(\Omega))$ and $u_0(a,x) \in L^2([0,A_m],\ V \cap W^{1,\infty}(\Omega))$, there exists a unique solution of (2.19) $u \in L^2((0,T] \times [0,A_m],\ V \cap W^{1,\infty}(\Omega))$.

Proof. We only need show the existence since Lemma 4 has already given the uniqueness. Like Lemma 4, we in fact only need show *(iii)* since *(i)* and *(ii)* can be obtained from this proof easily. Without loss of generality, we assume that $\mu \geq \lambda \gg 1$, otherwise, we only need consider the problem about $v = \exp(-\lambda t)u$ instead of u. We use a method involving the technique of delay $h > 0$. Let

$$P^h(t,x) = \begin{cases} P(t-h,x), & \text{if} \quad t \geq h \\ P(0,x), & \text{if} \quad t < h \end{cases} \tag{2.25}$$

where $P(t,x)$ is defined in the auxiliary population problem (III), i.e., (2.18). Also, assume that k^h , $\tilde{k}^h$ and μ^h are obtained from k , $\tilde{k}$ and μ by using P^h replacing P in k , $\tilde{k}$ and μ, respectively. We now consider the following delay problem,

$$\frac{\partial u^h}{\partial t}+\frac{\partial u^h}{\partial a}-\nabla\cdot(\tilde{k}^h\,\nabla u^h)= \ -\mu^h\ u^h \qquad \text{for } \forall\ t\in[0,T], a\in[0,A_m], x\in\Omega \tag{2.26}$$

$$\begin{aligned}
&\tilde{k}^h\frac{\partial u^h}{\partial\nu}=0 \quad\text{or}\quad u^h=0,\quad\text{on}\quad\partial\Omega\\
&u^h(0,a,x)= \ u_0(a,x)\\
&u^h(t,0,x)= \ B(t,\ x).
\end{aligned}\tag{2.27}$$

Its weak formulation is: Find $u^h:(0,T]\times[0,A_m]\longrightarrow V$, such that

$$\begin{aligned}
&(\partial_\tau\, u^h,\ w)+\alpha(\tilde{k}^h,\ u^h,\ w)=-(\mu^h u^h,\ w),\quad \text{for }\forall\ w\in V\\
&u^h(0,a,x)=u_0(a,\ x)\\
&u^h(t,0,x)= \ B(t,\ x).
\end{aligned}\tag{2.28}$$

It is not hard to see that the delay problem (2.26) (2.27) is linear over a *h-size* time interval. Hence, from partial differential equation theory and Lemma 2, we have that the problem (2.26)–(2.27) has a unique nonnegative weak solution $u^h\in L^2((0,T]\times[0,A_m],\ V\cap W^{1,\infty}(\Omega))$, that is, the problem (2.28) has a unique nonnegative solution. So, taking $w=u^h$ in (2.28), we obtain

$$\alpha(\tilde{k}^h,\ u^h,\ u^h)+(\mu^h u^h,\ u^h) \ = \ -(\partial_\tau\, u^h,\ u^h)$$

$$= -\frac{1}{2}\left(\frac{\partial(\|u^h\|_0^2)}{\partial t} + \frac{\partial(\|u^h\|_0^2)}{\partial a}\right).$$

Hence, by integrating over $[0,T] \times [0,A_m]$, it implies that

$$\int_0^T \int_0^{A_m} [\alpha(\tilde{k}^h,\ u^h,\ u^h) + (\mu^h u^h,\ u^h)]\, dt\, da$$

$$= -\frac{1}{2}\int_0^T \int_0^{A_m} \left(\frac{\partial(\|u^h\|_0^2)}{\partial t} + \frac{\partial(\|u^h\|_0^2)}{\partial a}\right) dt\, da$$

$$= \frac{1}{2}\int_0^{A_m} (\|u_0\|_0^2 - \|u^h(T,a,\cdot)\|_0^2\,)da + \frac{1}{2}\int_0^T (\,\|B\|_0^2 - \|u^h(t,A_m,\cdot)\|_0^2\,)dt$$

$$\leq \frac{1}{2}\int_0^{A_m} \|u_0\|_0^2\, da + \frac{1}{2}\int_0^T \|B\|_0^2 dt$$

$$\leq C(u_0, B).$$

Therefore, noting that (1.20) and $\mu \geq 1$, etc, we have

$$\int_0^T \int_0^{A_m} \|u^h\|_0^2\, dt\, da + k_1 \int_0^T \int_J^{A_m} \|\nabla u^h\|_0^2\, dt\, da$$

$$\leq \int_0^T \int_0^{A_m} [\alpha(\tilde{k}^h,\ u^h,\ u^h) + (\mu^h u^h,\ u^h)]\, dt\, da$$

$$\leq C(u_0, B) \tag{2.29}$$

On the other hand, notice that, for $a \in [0, J]$,

$$\begin{aligned} \frac{\partial u^h}{\partial t} + \frac{\partial u^h}{\partial a} = & -\mu^h u^h \\ & \text{for } \forall\, t \in (0, T], a \in [0, J], x \in \Omega. \end{aligned} \tag{2.30}$$

In fact, x in (2.30) can be regarded just as a parameter. So, from Lemma 1,

$$0 \leq u^h(t, a, x) \leq C(u_0, B), \quad \forall\, t \in (0, T], a \in [0, J], x \in \Omega.$$

Differentiating (2.30) with respect to a component of x, then we can have that

$$\frac{\partial u_x^h}{\partial t} + \frac{\partial u_x^h}{\partial a} = -\mu^h u_x^h - \partial\mu^h u^h$$

where u_x^h represents the first partial derivative of u^h and

$$\partial\mu^h = \frac{\partial\mu^h}{\partial x} + \frac{\partial\mu^h}{\partial P} P_x.$$

Therefore, we can have that

$$(\mu^h u_x^h,\ u_x^h) = -(\frac{\partial u_x^h}{\partial t},\ u_x^h) - (\frac{\partial u_x^h h}{\partial a},\ u_x^h) - (\partial\mu^h u^h,\ u_x^h)$$

$$-\int_0^T \int_0^J \left[(\frac{\partial u_x^h}{\partial t}, u_x^h) + (\frac{\partial u_x^h}{\partial a}, u_x^h) \right] dt\, da$$

$$= -\frac{1}{2} \int_0^T \int_0^J \left[\frac{\partial(\|u_x^h\|_0^2)}{\partial t} + \frac{\partial(\|u_x^h\|_0^2)}{\partial a} \right] dt\, da$$

$$= \frac{1}{2}\int_0^J (\|\frac{\partial u_0}{\partial x}\|_0^2 - \|u_x^h(T, a, \cdot)\|_0^2)da + \frac{1}{2}\int_0^T (\|\frac{\partial B}{\partial x}\|_0^2 - \|u_x^h(t, J, \cdot)\|_0^2)dt$$

$$\leq C(u_0, B)$$

and we can have that

$$\int_0^T \int_0^J |(\partial\mu^h\, u^h,\, u_x^h)\, |dt\, da$$

$$\leq C\int_0^T \int_0^J \int_\Omega |u^h|\, |u_x^h|(1 + |P_x^h|) dx\, dt\, da$$

$$\leq C(u_0, B)\int_0^T \int_0^J \int_\Omega |u_x^h|(1 + \int_0^{A_m} |u_x^h| da) dx\, dt\, da$$

$$\leq C(u_0, B) \left(\int_0^T \int_0^J \|u_x^h\|_0^2 dt\, da + \int_0^T \int_J^{A_m} |u_x^h|_0^2 dt\, da \right)$$

$$\leq C(u_0,B)\int_0^T \int_0^J \|u_x^h\|_0^2 dt\, da + C(u_0,B).$$

Hence, combining the above three estimates, we have that

$$\lambda\int_0^T \int_0^J |u_x^h|_0^2\, dt\, da \;\leq \int_0^T \int_0^J (\mu^h\, u_x^h,\; u_x^h)\, dt\, da$$

$$\leq C(u_0,B) + C(u_0,B) \int_0^T \int_0^J |u_x^h|_0^2\, dt\, da.$$

This, together with the choice of large enough λ, implies

$$\int_0^T \int_0^J |u^h|_1^2\, dt\, da \leq C(u_0,B). \tag{2.31}$$

Thus, (2.29) and (2.31) imply that

$$\int_0^T \int_0^{A_m} \|u^h\|_1^2\, dt\, da \leq C(u_0,B).$$

That means $\{u^h\}_h$ is uniformly bounded in the Hilbert spaces $L^2((0,T]\times[0,A_m],\ V)$. Hence, there exists a nonnegative $u \in L^2([0,T]\times[0,A_m],\ V)$ and a subsequence, for simplicity, still say $\{u^h\}_h$, such that the subsequence $\{u^h\}_h$ weakly converges to u as $h \to 0$, i.e.,

$$u^h \longrightarrow u, \quad \text{weakly in } L^2([0,T]\times[0,A_m],\ V) \quad \text{as } h \to 0\,.$$

We also can have that

$$P^h \longrightarrow P, \quad \text{weakly in } L^2([0,T],\ V) \quad \text{as} \quad h \to 0$$
$$\alpha(\tilde{k}^h,\ u^h,\ w) \longrightarrow \alpha(\tilde{k},\ u,\ w), \quad \text{as} \quad h \to 0, \quad \forall\, w \in V$$
$$(\,\mu^h u^h,\ w) \longrightarrow (\,\mu\, u,\ w), \quad \text{as} \quad h \to 0, \quad \forall\, w \in V.$$

For (2.32) with the subsequence $\{u^h\}_h$, letting $h \to 0$, we then get

$$\begin{aligned} &(\partial_\tau u,\ w) + \alpha(\tilde{k},\ u,\ w) = -(\mu u,\ w), \quad \text{for } \forall\, w \in V \\ &u(0,a,x) = u_0(a,\ x) \\ &u(t,0,x) = B(t,\ x). \end{aligned} \tag{2.32}$$

This means that $u \in L^2((0,T] \times [0,A_m],\ V)$ is a solution of (2.32). Moreover, from the regularity theory of partial differential problem and Lemma 1 and Lemma 2 of this section, we have that $u \in L^2([0,T] \times [0,A_m], \cap W^{1,\infty}(\Omega))$. Therefore, such a solution u is unique from Lemma 2 and 3 of this section. Finally, we would like to mention that, by a standard argument of functional analysis (cf. [34, 75, 117]), we can show that the whole sequence $\{u^h\}_h$ is strongly convergent to u in the sense of $L^2([0,T] \times [0,A_m],\ V)$. This has finished the proof.

Consider the case for which $B(t,x)$ is replaced by renewal equation, i.e.,

$$\begin{aligned} &\frac{\partial u}{\partial t} + \frac{\partial u}{\partial a} - \nabla \cdot (\tilde{k}\,\nabla u) = -\mu\, u \\ &\qquad\qquad \text{for } \forall\; t \in [0,T], a \in [0,A_m], x \in \Omega \end{aligned} \tag{2.33}$$

$$\begin{aligned} &\tilde{k}\frac{\partial u}{\partial \nu} = 0 \ \text{ or } \quad u = 0, \ \ x \in \partial\Omega \\ &u(0,a,x) = \ u_0(a,x) \\ &u(t,0,x) = \int_0^\infty \beta\, u(t,a,x)\, da \end{aligned} \tag{2.34}$$

where $\beta = \beta(t,a,x,P)$ is the birth rate. Its corresponding weak form is: Find $u : (0,T] \times [0,A_m] \longrightarrow V$, such that

$$\begin{aligned} &(\partial_\tau\, u,\ w) + \alpha(\tilde{k},\ u,\ w) = -(\mu u,\ w), \quad \text{for } \forall\ w \in V \\ &u(0,a,x) = u_0(a,\ x) \\ &u(t,0,x) = \int_0^{A_m} \beta u(t,a,x) da. \end{aligned} \tag{2.35}$$

THEOREM 2 *Assume that μ is a nonnegative continuous function and has bounded first derivatives with respect to all of its variables. Also assume that k and β are nonnegative continuous function and has a bounded first derivative with respect to P, that is,*

$$\begin{aligned} &k_2 \ \geq \ k \ \geq \ k_1 \ > \ 0, \quad |\frac{\partial k}{\partial P}| \leq C_k \\ &\bar{\beta} \geq \beta \geq 0, \ \ |\frac{\partial \beta}{\partial P}| \leq C_\beta \end{aligned}$$

where k_1, k_2, $\bar{\beta}$, C_k and C_β are constants. Let $u_0(a,x) \in L^2([0,A_m],\ V)$ be given. Then

(i) if both k, μ and β are independent of P, there exists at most one weak solution of (2.35).

(ii) if k is independent of P, $u_0(a,x) \in L^2([0,A_m],\ V \cap L^\infty(\Omega)\,)$, there exists

at most one solution of (2.35) $u \in L^2((0,T] \times [0,A_m],\ V \cap L^\infty(\Omega)\,)$.

(iii) if $u_0(a,x) \in L^2([0,A_m],\ V \cap W^{1,\infty}(\Omega))$, *there exists at most one solution of* (2.35) $u \in L^2((0,T] \times [0,A_m],\ V \cap W^{1,\infty}(\Omega)\,)$.

Proof. Like the previous lemma and Theorem, we only show *(iii)*. Similar to the argument in the proof of Lemma 4, let $u_1,\ u_2 \in L^2([0,A_m],\ V \cap W^{1,\infty}(\Omega)\,)$ be two weak solutions of (2.35). Also, we introduce a parameter $\lambda \gg 1$ and adopt (2.20) – (2.21), in particular,

$$w = v_1 - v_2 = \exp(-\lambda\, t)(u_1 - u_2).$$

Then, we can have from (2.35) that

$$w(0,a,x) = 0, \quad \text{for} \quad a \in [0,A_m], \quad x \in \Omega \tag{2.36}$$

$$w(t,0,x) = \int_0^{A_m} (\beta^*(P_1)\, v_1 - \beta^*(P_2)\, v_2)\, da \tag{2.37}$$

where β^* is understood same as in the proof of Lemma 4. Also, for v_i $(i = 1,2)$, we can have that

$$(\partial_\tau\, v_i,\ w) + \alpha(\tilde{k}^*(P_i),\ u,\ w) + (\,(\mu^*(p_i) + \lambda)\, v_i,\ w) = 0.$$

Hence,

$$
\begin{aligned}
&(\partial_\tau w,\, w) + (\, \alpha(\tilde{k}^*(P_1),\, v_1,\, w) - \alpha(\tilde{k}^*(P_2),\, v_2,\, w)\,) \\
&\quad + (\, (\mu^*(P_1)\, v_1,\ w) - (\mu^*(P_2)\, v_1,\ w)\,) + \lambda(w,\, w) = 0\,.
\end{aligned}
\tag{2.38}
$$

By a direct computation, we obtain that from (2.20) – (2.21), etc.

$$
\begin{aligned}
&\int_0^T \int_0^{A_m} (\partial_\tau w,\, w)\, dt\, da \\
= \;& \frac{1}{2}\int_0^T \int_0^{A_m} \left[\frac{\partial(\|w\|_0^2)}{\partial t} + \frac{\partial(\|w\|_0^2)}{\partial a}\right] dt\, da \\
= \;& \frac{1}{2}\left[\int_0^T \left(\, \|w(t, A_m, \cdot)\|_0^2 - \|w(t, 0, \cdot)\|_0^2\,\right)\, dt + \int_0^{A_m} \|w(T, a,, \cdot)\|_0^2\, da\right] \\
\geq \;& -\frac{1}{2}\int_0^T \|w(t, 0, \cdot)\|_0^2\, dt \\
\geq \;& -\int_0^T \int_\Omega \left(\int_0^{A_m} (\beta^*(P_1)\, v_1 - \beta^*(P_2)\, v_2)\, da\right)^2 dx dt \\
\geq \;& -A_m \int_0^T \int_0^{A_m} \int_\Omega (\beta^*(P_1)\, v_1 - \beta^*(P_2)\, v_2)^2 dx\, dt\, da \\
\geq \;& -A_m \int_0^T \int_0^{A_m} \int_\Omega (\bar{\beta}|w|^2 + |\beta^*(P_1) - \beta^*(P_2)| \cdot |v_2|)\, dt\, da
\end{aligned}
$$

$$\geq -C\int_0^T \int_0^{A_m} \int_\Omega (|w|^2 + C_\beta |v_1 - v_2| \cdot |u_2|)dx\, dt\, da$$

$$\geq -C(A_m, \bar{\beta}, C_\beta, M)\int_0^T \int_0^{A_m} \|w\|_0^2\, dt\, da. \tag{2.39}$$

Therefore, it follows from (2.23) (2.24) and (2.38) (2.39) that

$$\begin{aligned} 0 &= \int_0^T \int_0^{A_m} [(\partial_\tau w,\ w) + (\ \alpha(\tilde{k}^*(P_1),\ v_1,\ w) - \alpha(\tilde{k}^*(P_2),\ v_2,\ w)\ ) \\ &\qquad +(\ (\mu^*(P_1)\, v_1,\ w) - (\mu^*(P_2)\, v_1,\ w)\ ) + \lambda(w,\ w)]dt\, da \\ &\geq (\lambda - C))\int_0^T \int_0^{A_m} \|w\|_0^2\, dt\, da. \end{aligned}$$

Thus, by taking λ large enough, this implies that

$$\int_0^T \int_0^{A_m} \|w\|_0^2\, dt\, da \leq 0.$$

Hence, we have proved this uniqueness theorem.

We now consider the existence for problem (2.35) (or (2.33) (2.34)). We first consider a simple case in which we assume that k, μ and β are all independent of P. We use a fixed point technique to show the following theorem.

THEOREM 3 *Assume that the assumptions of Theorem* 2 *(i) hold and let*

$$\beta = 0, \quad \textit{for} \quad \forall t \in [0,T],\ a \in [0,J],\ x \in \Omega.$$

Then there exists a unique nonnegative weak solution satisfying (2.35).

Proof. Notice that the problem of this case is just a special situation of the problem in Theorem 2, so, we can directly have the uniqueness from Theorem 2. However, observing the proof of Theorem 2, we in fact obtain a stronger result, a uniqueness in $L^2((0,T]\times[0,A_m],\ V)$, only requiring a weaker condition, $u_0\in L^2([0,A_m],\ V)$.

We now consider the existence. Like in the proof of Theorem 1, without loss of generality, we assume that $\mu\geq\lambda\gg 1$. Let

$$\mathcal{H}=(\{u\geq 0\})\cap L^2((0,T]\times[0,A_m],\ L^2(\Omega))\cap L^2((0,T]\times[J,A_m],\ V). \quad (2.40)$$

Clearly, $\mathcal{H}$ is a closed convex set of a Hilbert space. For $v\in\mathcal{H}$, we consider the the following auxiliary problem: Find $u:(0,T]\times[0,A_m]\longrightarrow V$, such that

$$\begin{aligned}&(\partial_\tau u,\ w)+\alpha(\tilde{k},\ u,\ w)=-(\mu u,\ w),\quad \text{for } \forall\, w\in V\\ &u(0,a,x)=u_0(a,\ x)\\ &u(t,0,x)=\ B(t,x)\equiv\int_0^{A_m}\beta\, v\, da.\end{aligned} \quad (2.41)$$

Notice that, while $v\in\mathcal{H}$ is given, $B(t,x)$ is known and k, μ and β are all independent of P. Therefore, (2.41) is clearly a linear problem. It then is easy to see that $B\in L^2((0,T],\ V)$. Then, it follows from Lemma 4 and Theorem 1 that the problem (2.41) has a unique solution $u\in L^2((0,T]\times[0,A_m],\ V)$.

Therefore, we can define a mapping: $\mathbf{T} : \mathcal{H} \longrightarrow \mathcal{H}$, such that $\mathbf{T}v = u$, where u is the above unique solution of (2.41). We are now left with showing that $\mathbf{T}$ is strictly contracting.

Let $v_1, \ v_2 \ \in \mathcal{H}$ be two elements of $\mathcal{H}$ and let $u_i = \mathbf{T}\, v_i, \ (i = 1, 2)$. Then we have that from (2.41)

$$\begin{aligned} (\, u_1 \ - \ u_2\,)\,|_{t=0} \ &= \ 0 \\ (\, u_1 \ - \ u_2\,)\,|_{a=0} \ &= \ \int_0^{A_m} \beta(v_1 - v_2)\, da \end{aligned}$$

$$(\partial_\tau(u_1 - u_2),\ w) + \alpha(\tilde{k}, u_1 - u_2, w) + (\mu\,(u_1 - u_2),\ w) = 0$$
$$\forall\, w \in V, \ \ t \ \in \ (0, T], \ \ a \ \in \ [0, A_m].$$

Taking $w = u_1 - u_2$ in the above formulation and then integrating it over $[0, T] \times [0, A_m]$, we can obtain

$$k_1 \int_0^T \int_J^{A_m} |u_1 - u_2|_1^2 \, dt\, da + \lambda \int_0^T \int_0^{A_m} \|u_1 - u_2\|_0^2 \, dt\, da$$

$$\leq \int_0^T \int_J^{A_m} \left[\alpha(\tilde{k}, u_1 - u_2,\ u_1 - u_2) + (\mu\,(u_1 - u_2),\ u_1 - u_2)\right]\, dt\, da$$

$$\leq - \int_0^T \int_0^{A_m} (\partial_\tau(u_1 - u_2),\ u_1 - u_2)\, dt\, da. \tag{2.42}$$

By a direct computation, we obtain that

$$\int_0^T \int_0^{A_m} \left(\partial_\tau(u_1 - u_2),\; u_1 - u_2 \right) \, dt \, da$$

$$= \frac{1}{2}\int_0^T \int_0^{A_m} \left[\frac{\partial(\|u_1 - u_2\|_0^2)}{\partial t} + \frac{\partial(\|u_1 - u_2\|_0^2)}{\partial a} \right] dt \, da$$

$$\geq -\frac{1}{2}\int_0^T (\|u_1 - u_2\|_0^2) \,|_{a=0} \; dt$$

$$= -\frac{1}{2}\int_0^T \int_\Omega \left[\int_0^{A_m} \beta(v_1 - v_2) \, da \right]^2 dx \, dt$$

$$\geq -\frac{1}{2} A_m \bar{\beta}^2 \int_0^T \int_\Omega \int_0^{A_m} |v_1 - v_2| \, da \, dx \, dt$$

$$\geq -C\int_0^T \int_0^{A_m} \|v_1 - v_2\|_0^2 \, dt \, da.$$

Thus, this, together with (2.42), implies that

$$k_1\int_0^T \int_J^{A_m} |\mathbf{T}v_1 - \mathbf{T}v_2|_1^2 \, dt \, da + \lambda\int_0^T \int_0^{A_m} \|\mathbf{T}v_1 - \mathbf{T}v_2\|_0^2 \, dt \, da$$

$$= \; k_1\int_0^T \int_J^{A_m} |u_1 - u_2|_1^2 \, dt \, da + \lambda\int_0^T \int_0^{A_m} \|u_1 - u_2\|_0^2 \, dt \, da$$

$$\leq C\int_0^T \int_0^{A_m} \|v_1 - v_2\|_0^2 \, dt \, da.$$

Therefore, we can deduce that T is a strict contraction when λ is large enough. Thus, there exists a $u \in \mathcal{H}$, a fixed point of T. This and Theorem 1 indicate that $u \in \mathcal{H}$ is the solution of (2.35). We then have completed the proof.

Finally, we have one of the main results in this section obtained by the delay technique as for Theorem 1.

THEOREM 4 *Assume that μ is a nonnegative continuous function and has bounded first derivatives with respect to all of its variables. Also assume that k and β are nonnegative continuous functions and have a bounded first derivative with respect to P, that is,*

$$\begin{aligned}
&k_2 \geq k \geq k_1 > 0, \quad |\frac{\partial k}{\partial P}| \leq C_k \\
&\bar{\beta} \geq \beta \geq 0, \quad |\frac{\partial \beta}{\partial P}| \leq C_\beta \\
&\beta = 0, \quad \text{for} \quad \forall t \in [0,T], \ a \in [0,J], \ x \in \Omega
\end{aligned}$$

where k_1, k_2, $\bar{\beta}$, C_k and C_β are constants. Let $u_0(a,x) \in L^2([0,A_m],\ V)$ be given. Then we have

(i) if both k, μ and β are independent of P, there exists a unique weak solution of (2.35).

(ii) if k is independent of P, $u_0(a,x) \in L^2([0,A_m],\ V \cap L^\infty(\Omega)\,)$, there exists a unique solution of (2.35) $u \in L^2((0,T] \times [0,A_m],\ V \cap L^\infty(\Omega)\,)$.

(iii) if $u_0(a,x) \in L^2([0,A_m],\ V \cap W^{1,\infty}(\Omega)\,)$, there exists a unique solution of

(2.35) $u \in L^2((0,T] \times [0, A_m],\ V \cap W^{1,\infty}(\Omega))$.

Proof. Like the previous Lemmas and Theorems of this section, we only need discuss (*iii*). Similar to the proof of Theorem 1, without loss of generality, we assume that $\mu \geq \lambda \gg 1$. For $h \geq 0$, a delay, we introduce P^h as in (2.25) in the proof of Theorem 1 and adopt some related notations, for instance, k^h, $\tilde{k}^h$ and μ^h, etc. Also, we similarly introduce $\beta^h = \beta(t, a, x, P^h)$. We now consider the delay problem as follows.

$$\begin{gathered}\frac{\partial u^h}{\partial t} + \frac{\partial u^h}{\partial a} - \nabla \cdot (\tilde{k}^h \nabla u^h) = -\mu^h u^h \\ \text{for } \forall\, t \in (0,T], a \in [0, A_m], x \in \Omega\end{gathered} \tag{2.43}$$

$$\begin{aligned}&\tilde{k}^h \frac{\partial u^h}{\partial \nu} = 0 \quad \text{or} \quad u^h = 0, \quad \text{on} \quad \partial\Omega \\ &u^h(0, a, x) = u_0(a, x), \\ &u^h(t, 0, x) = \int_0^\infty \beta^h u^h(t, a, x)\, da.\end{aligned} \tag{2.44}$$

Its weak formulation is: Find $u^h : (0,T] \times [0, A_m] \longrightarrow V$, such that

$$\begin{aligned}&(\partial_\tau u^h,\ w) + \alpha(\tilde{k}^h,\ u^h,\ w) = -(\mu^h u^h,\ w), \quad \text{for } \forall\, w \in V \\ &u^h(0, a, x) = u_0(a,\ x) \\ &u^h(t, 0, x) = \int_0^\infty \beta^h u^h(t, a, x)\, da.\end{aligned} \tag{2.45}$$

Clearly, the delay problem (2.45) is linear over a *h-size* time interval. It follows from Theorem 3 that the delay problem (2.45) has a unique nonegative solution

$u^h \in L^2([0,T] \times [0,A_m],\ V)$. Taking $w = u^h$ in (2.45), we obtain

$$\begin{aligned} \alpha(\tilde{k}^h,\ u^h,\ u^h) + (\mu^h u^h,\ u^h) &= -(\partial_\tau\, u^h,\ u^h) \\ &= -\frac{1}{2}\left(\frac{\partial(\|u^h\|_0^2)}{\partial t} + \frac{\partial(\|u^h\|_0^2)}{\partial a}\right). \end{aligned} \tag{2.46}$$

By elementary computations, we obtain

$$\begin{aligned} &-\frac{1}{2}\int_0^T \int_0^{A_m} \left[\frac{\partial(\|u^h\|_0^2)}{\partial t} + \frac{\partial(\|u^h\|_0^2)}{\partial a}\right] dt\, da \\ &\leq \frac{1}{2}\int_0^{A_m} \|u_0\|_0^2\, da + \frac{1}{2}\int_0^T \|u^h(t,0,x)\|_0^2\, dt \\ &\leq C(u_0) + \tfrac{A_m}{2}\int_0^T \int_\Omega \int_0^{A_m} (\beta\, u^h)^2\, da\, dx\, dt \\ &\leq C(u_0) + A_m\, \bar{\beta}^2 \int_0^T \int_0^{A_m} \|u\|_0^2\, dt\, da. \end{aligned}$$

This, together with (2.46) and $\mu \geq \lambda \gg 1$, indicates that

$$\begin{aligned} &\int_0^T \int_0^{A_m} \|u^h\|_0^2\, dt\, da + k_1 \int_0^T \int_J^{A_m} \|\nabla u^h\|_0^2\, dt\, da \\ &\leq \lambda \int_0^T \int_0^{A_m} \|u^h\|_0^2\, dt\, da + k_1 \int_0^T \int_J^{A_m} \|\nabla u^h\|_0^2\, dt\, da \end{aligned}$$

$$\leq \int_0^T \int_0^{A_m} \left[\alpha(\tilde{k}^h,\ u^h,\ u^h) + (\mu^h u^h,\ u^h) \right] dt\, da$$

$$= -\frac{1}{2} \int_0^T \int_0^{A_m} \left[\frac{\partial(\|u^h\|_0^2)}{\partial t} + \frac{\partial(\|u^h\|_0^2)}{\partial a} \right] dt\, da$$

$$\leq C(u_0) + A_m\, \bar{\beta}^2 \int_0^T \int_0^{A_m} \|u\|_0^2\, dt\, da$$

$$\leq C(u_0, A_m, \beta). \tag{2.47}$$

On the other hand, by a completely similar argument as that between (2.30) and (2.31), we have that (using the same notations)

$$(\mu^h\, u_x^h,\ u_x^h) = -\frac{1}{2} \left[\frac{\partial(\|u_x^h\|_0^2)}{\partial t} + \frac{\partial(\|u_x^h\|_0^2)}{\partial a} \right] - (\partial\mu^h\, u^h,\ u_x^h) \tag{2.48}$$

$$-\frac{1}{2} \int_0^T \int_0^J \left[\frac{\partial(\|u_x^h\|_0^2)}{\partial t} + \frac{\partial(\|u_x^h\|_0^2)}{\partial a} \right] dt\, da$$

$$\leq \frac{1}{2} \int_0^J \left(\|\frac{\partial u_0}{\partial x}\|_0^2 - \|u_x^h(T, a, x)\|_0^2 \right) da + \frac{1}{2} \int_0^T \left(\|u_x^h(t, 0, x)\|_0^2 - \|u_x^h(t, J, x)\|_0^2 \right) dt$$

$$\leq \frac{1}{2} \int_0^J \|\frac{\partial u_0}{\partial x}\|_0^2\, da + \frac{1}{2} \int_0^T \|u_x^h(t, 0, x)\|_0^2\, dt$$

$$\leq C(u_0) + \int_0^T \int_\Omega \left[\int_0^{A_m} \beta \, u_x^h \, da \right]^2 dx \, dt$$

$$\leq C(u_0) + A_m \int_0^T \int_\Omega \left[\int_J^{A_m} (\beta \, u_x^h)^2 da \right]^2 dx \, dt$$

$$\leq C(u_0) + A_m \, \bar{\beta}^2 \int_0^T \int_J^{A_m} |u_x^h|_0^2 \, dt \, da$$

$$\leq C(u_0, A_m, \beta)$$

and

$$\int_0^T \int_0^J |(\partial \mu^h \, u^h, \; u_x^h) \, | \, dt \, da$$

$$\leq C(u_0, A_m, \beta) \int_0^T \int_0^J \|u_x^h\|_0^2 \, dt \, da + C(u_0, A_m, \beta).$$

Combining the above three estimates and noting that $\mu \geq \lambda \gg 1$, we obtain

$$\begin{aligned} \int_0^T \int_0^J \|u_x^h\|_0^2 \, dt \, da &\leq \lambda \int_0^T \int_0^J |u_x^h|_0^2 \, dt \, da \\ &\leq \int_0^T \int_0^J (\mu^h \, u_x^h, \; u_x^h) \, dt \, da \\ &\leq C(u_0, A_m, \beta) \int_0^T \int_0^J \|u_x^h\|_0^2 dt \, da + C(u_0, A_m, \beta) \end{aligned}$$

$$\leq \; C(u_0, A_m, \beta).$$

This, together with (2.47), implies

$$\int_0^T \int_0^{A_m} \|u^h\|_1^2 \, dt \, da \leq C(u_0, A_m, \beta). \tag{2.49}$$

Hence, there exists a nonnegative $u \in L^2((0,T] \times [0, A_m], \; V)$ and a subsequence, for simplicity, still say $\{u^h\}_h$, such that the subsequence $\{u^h\}_h$ weakly converges to u as $h \to 0$, i.e.,

$$u^h \longrightarrow u, \quad \text{weakly in } L^2((0,T] \times [0, A_m], \; V) \quad \text{as } h \to 0\,.$$

We can have that by a direct computation

$$\begin{aligned}
&P^h \longrightarrow P, \quad \text{weakly in } L^2((0,T], \; V) \quad \text{as } h \to 0 \\
&\alpha(\tilde{k}^h, \; u^h, \; w) \longrightarrow \alpha(\tilde{k}, \; u, \; w), \quad \text{as } h \to 0, \quad \forall\, w \in V \\
&(\,\mu^h\, u^h, \; w) \; \longrightarrow \; (\,\mu\, u, \; w), \quad \text{as } h \to 0, \quad \forall\, w \in V.
\end{aligned}$$

Also, we have that, as $h \to 0$,

$$\int_0^{A_m} \beta^h \, u^h(t, a, x) \, da \longrightarrow \int_0^{A_m} \beta \, u(t, a, x) \, da.$$

For the delay problem (2.45) with the subsequence $\{u^h\}_h$, by letting $h \to 0$, we then have that

$$
\begin{aligned}
&(\partial_\tau u,\ w) + \alpha(\tilde{k},\ u,\ w) = -(\mu\, u,\ w), \quad \text{for } \forall\ w \in V \\
&u(0,a,x) = u_0(a,\ x) \\
&u(t,0,x) = \int_0^{A_m} \beta u(t,a,x) da.
\end{aligned}
$$

This means that $u \in L^2((0,T] \times [0,A_m],\ V)$ is a nonnegative weak solution of (2.35). Thus, we have proved the Theorem 4.

Remark 2.3.1: If we replace $k\nabla u$ by $k\nabla u - \mathbf{q}u$ in the auxiliary age structured population problem (II), that is, we consider the model with both diffusion and advection, then the corresponding bilinear form becomes as

$$\alpha(k,u,v) - (\mathbf{q}\, u,\ v) + (\mu\, u,\ v). \tag{2.50}$$

Clearly, the bilinear form (2.50) is not symmetric. However, as we have indicated in Lemma 4 and Theorem 1- 4, we can assume that, without loss of the generality, $\mu > \lambda$ (*constant*) is large enough. This means, we may always assume that the bilinear form (2.50) is coercive. Otherwise, we can apply a simple transformation as in the proofs of Lemma 4 and Theorem 1- 4, then we obtain a similar problem but with a coercive bilinear form like (2.50). Therefore, from the related analyses and proofs about Lemma 2 and Lemma 3 in [89, 78, 115, 114], it is not hard to show that Lemma 2 and Lemma 3 are still true for the model with both diffusion and advection.

Remark 2.3.2: From **Remark 2.3.1** and the proofs of Lemma 4 and Theorem 1– 4, it is not very hard to show that Lemma 4 and Theorem 1– 4 can be extended to the model like *Mixed Age Structured Population Problem (III)* but with both diffusion and advection in the older life stage. More precisely, If the term $\tilde{k}\nabla u$ in (2.18) and (2.33) is replaced by the term $\nabla u - \tilde{\mathbf{q}}\, u$, we then can show that Lemma 4 and Theorem 1– 4 are still true for the model like *Mixed Age Structured Population Problem (III)* but with both diffusion and advection in the older life stage.

2.3 Mathematical Treatments

In this section, we present a primary mathematical analysis for the mathematical model for individual-based, physiological structured fish populations in a spatially heterogenous environment, which is proposed in the previous sections and Chapter 1. This mathematical model consists of two parts: individual model and individual-based population dynamic model. In biology, this is a structured model. This is a very complicated and difficult problem, which is a mixed problem of a initial value problem of ordinary differential system, an individual fish model, and a nonlocal initial-boundary value partial differential equation problem, a population dynamic model. In particular, the partial differential problem is indeed a differential–integral problem with a discontinuous coefficient. The discontinuous coefficient is coupled with a quasi-linear hyperbolic equation and a degenerate parabolic equation. The study methodology is to apply a localization technique, an unstructuralization technique for physiological structures, and a linearization technique to change the original complicated mathematical problem into a sequence of age structured and linear (approximation) problem over a set of small time (age) intervals. Thus, we may use the methods and results of the previous sections to analyze them. Moreover, notice that the analysis is constructive, so it may be applied to construct the approximation scheme. In fact, this is just the basic idea to construct the computational model for an individual-based fish population model in a heterogenous (chemical toxicant) environment discussed in the next chapter.

We first consider the individual model which is an initial value problem for an ordinary differential system with two equations if without chemical toxicant effects, or three equations if with chemical toxicant effects:

Individual Model:

$$\begin{aligned} \frac{dm_L}{da} &\equiv g_L = G_L - F_L \\ \frac{dm_S}{da} &\equiv g_S = G_S - F_S \end{aligned} \tag{2.51}$$

$$
\begin{aligned}
m_L|_{a=a_0} &= m_{L_0} \\
m_S|_{a=a_0} &= m_{S_0}
\end{aligned}
\tag{2.52}
$$

Individual Model with Toxicant Effects:

$$
\begin{aligned}
\frac{dm_L}{da} &\equiv g_L = \chi G_L - F_L \\
\frac{dm_S}{da} &\equiv g_S = \chi G_S - F_S
\end{aligned}
\tag{2.53}
$$

$$
\begin{aligned}
m_L|_{a=a_0} &= m_{L_0} \\
m_S|_{a=a_0} &= m_{S_0}
\end{aligned}
\tag{2.54}
$$

$$
\begin{aligned}
\frac{dB_T}{da} &\equiv g_c = sk_w C_w + C_F F - \frac{B_T}{W_T BCF}(sk_w + Ek_E) \\
B_T|_{a=a_0} &= B_{T_0}
\end{aligned}
\tag{2.55}
$$

Therefore, we can have the following existence results (cf. [76, 90]).

PROPOSITION 1 *There is a* $\tau > 0$*, such that both problem* (2.51) - (2.52) *and problem* (2.53)–(2.55) *have a unique solution in* $[a_0, a_0 + \tau]$.

We have shown that, except for the above individual model, the mathematical model for individual-based population model includes the following population dynamic model, which is proposed in Section 1 of this chapter.

Population Dynamics Model:

$$\begin{aligned}\frac{\partial \rho}{\partial t}+\frac{\partial \rho}{\partial a}+\frac{\partial(\rho\, g_L)}{\partial m_L}+\frac{\partial(\rho\, g_S)}{\partial m_S} &= \; -\mu\rho \\ &\text{for } t\in(0,T], a\in(0,J], x\in\Omega\end{aligned} \tag{2.56}$$

$$\begin{aligned}\frac{\partial \rho}{\partial t}+\frac{\partial \rho}{\partial a}+\frac{\partial(\rho\, g_L)}{\partial m_L}+\frac{\partial(\rho\, g_S)}{\partial m_S}-\nabla\cdot(k\nabla\rho) &= \; -\mu\rho \\ &\text{for } t\in(0,T], a\in(J,A_m], x\in\Omega\end{aligned} \tag{2.57}$$

$$\begin{aligned}& k\frac{\partial \rho}{\partial \nu}=0 \quad \text{or} \quad \rho=0, \quad \text{on } \partial\Omega \\ & \rho\,|_{t=0} \; = \; \rho_0(a,m_L,m_S,x) \\ & \rho(t,0,m_{L_0},m_{S_0},x) = \; \int_0^{A_m}\int_0^\infty\int_0^\infty \beta\rho(t,a,m_L,m_S,x)\, da\, dm_L\, dm_S\end{aligned}$$

Moreover, extending k to $\tilde{k}$ defined in (1.20), we can rewrite the above population dynamic model as follows.

$$\begin{aligned}\frac{\partial \rho}{\partial t}+\frac{\partial \rho}{\partial a}+\frac{\partial(\rho\, g_L)}{\partial m_L}+\frac{\partial(\rho\, g_S)}{\partial m_S}-\nabla\cdot(\tilde{k}\,\nabla\rho) &= \; -\mu\rho \\ &\text{for } t\in(0,T], a\in[0,A_m], x\in\Omega\end{aligned} \tag{2.58}$$

$$\begin{aligned}& \tilde{k}\,\frac{\partial \rho}{\partial \nu}=0 \quad \text{or} \quad \rho=0, \quad \text{on } \partial\Omega \\ & \rho\,|_{t=0} \; = \; \rho_0(a,m_L,m_S,x) \\ & \rho(t,0,m_{L_0},m_{S_0},x) = \int_0^{A_m}\int_0^\infty\int_0^\infty \beta\rho(t,a,m_L,m_S,x) da dm_L dm_S\end{aligned} \tag{2.59}$$

Notice that we suppose that, for fish, n tasks (feeding, reproduction, movement, etc.) are accomplished sequentially. Thus, from biological point of view, it is reasonable to solve the individual model (that is, calculate the growth of fish) first and then consider the change in population distribution (that is, reproduction, movement, etc) in a small time (age) interval. In mathematics, while the individual model is solved first in a small time (age) interval, we can plug the solution of the individual model into the population dynamics model of the small time (age) interval since the coupled relation between the ordinary differential system, which describes the individual model, and the partial differential problems, which describes the population dynamics models, is a weak association. Hence, after plugging in the solution of the individual model, the population dynamics in the small time (age) interval becomes physiological structure free. That means we locally unstructuralize the physiological structures in the population dynamics model. Therefore, we may apply the results and methods, for example, local linearization technique and the method involving a *h-delay* ($h > 0$), for the age structured population model to analyze it. So, clearly we have to discuss the local solution problem for our model first in order to discuss the global problem by using the above strategy. If there is a local solution on small time (age) intervals, then we may use these local solutions to construct a global (at least approximate) solution.

Let J_0 be a small time interval. For some initial condition, we solve the individual model (2.51) or (2.53) over J_0 and obtain the solution $(\widetilde{m}_L,\ \widetilde{m}_S)$. Plugging this $(\widetilde{m}_L,\ \widetilde{m}_S)$ into the population dynamics model (2.56) - (2.59), we have that

$$\widetilde{\rho}(t,a,x) = \rho(t,a,\widetilde{m}_L,\ \widetilde{m}_S,x). \tag{2.60}$$

By elementary computation, we obtain that

$$\frac{\partial \widetilde{\rho}}{\partial t} = \frac{\partial \rho}{\partial t}$$

$$\frac{\partial \widetilde{\rho}}{\partial a} = \frac{\partial \rho}{\partial a} + \frac{\partial \rho}{\partial m_L}\, g_L + \frac{\partial \rho}{\partial m_S}\, g_S$$

so,

$$\begin{aligned} \frac{\partial \widetilde{\rho}}{\partial t} + \frac{\partial \widetilde{\rho}}{\partial a} &= \frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial a} + \frac{\partial(\rho\, g_L)}{\partial m_L} + \frac{\partial(\rho\, g_S)}{\partial m_S} \\ &\quad - \frac{\partial g_L}{\partial m_L}\,\rho - \frac{\partial g_S}{\partial m_S}\,\rho \end{aligned} \tag{2.61}$$

if we do not change the notations for μ, k, $\tilde{k}$, and β after replacing m_L and m_S by $\widetilde{m}_L$ and $\widetilde{m}_S$, then the population dynamics model (2.58) – (2.59) becomes a partial differential problem for $\widetilde{\rho}$ as follows.

$$\frac{\partial \widetilde{\rho}}{\partial t} + \frac{\partial \widetilde{\rho}}{\partial a} - \nabla\cdot(\tilde{k}\nabla\widetilde{\rho}) = -(\mu + \frac{\partial g_L}{\partial m_L} + \frac{\partial g_S}{\partial m_S})\cdot\widetilde{\rho} \tag{2.62}$$

$$t \in\ J_0, \quad a \in [0, A_m], \quad x \in \Omega$$

$$\begin{aligned} &\tilde{k}\frac{\partial \tilde{\rho}}{\partial \nu} = 0 \quad \text{or} \quad \tilde{\rho} = 0, \quad \text{on} \quad \partial\Omega \\ &\tilde{\rho}\mid_{t=t_0} \quad (given) \\ &\tilde{\rho}\mid_{a=0} = \int_0^{A_m}\int_0^{\infty}\int_0^{\infty} \beta\tilde{\rho}\, da. \end{aligned} \tag{2.63}$$

Clearly, (2.62)–(2.63) is unstructured. This means we have locally unstructurized (2.58)–(2.59) over the small time interval J_0. Therefore, we can use the techniques of linearization and delay, etc. of last section or directly use the results of Theorem 4 of last section to show that (2.62)–(2.63) has a weak solution. That is, there exists a $\tilde{\rho} \in L^2(J_0 \times [0, A_m],\ V)$ which satisfies the initial-boundary condition (2.63) and

$$\begin{aligned} (\frac{\partial \tilde{\rho}}{\partial t} + \frac{\partial \tilde{\rho}}{\partial a},\ w) + \alpha(\tilde{k},\ \tilde{\rho},\ w) = -((\mu + \frac{\partial g_L}{\partial m_L} + \frac{\partial g_S}{\partial m_S})\,\tilde{\rho}, w) \\ \forall w \in V, \quad t \in J_0, \quad a \in [0, T]. \end{aligned} \tag{2.64}$$

Then we have

PROPOSITION 2 *Assume that k, μ and β satisfy the conditions in Theorem 4. For $t_0 \geq 0$, if $\rho\mid_{t=t_0} \in L^2([0, A_m], V)$, then the mathematical model for individual-based fish populations has a local weak solution.*

We here only give a outline about constructing global solution since it is useful for us to construct the numerical schemes next chapter. However, we don't give any details and we plan to show it elsewhere since it is very complicated. The basic procedure of this method can be described as follows. For $h > 0$, we divide the time domain into a set of *h-size* small interval $[t_i, t_{i+1}]$, $t_i = i * h$, $i = 0, 1, \cdots$. Then, from the above proposition, we could at least obtain an approximate local solution on each small time interval $[t_i, t_{i+1}]$ in order $i = 0, 1, 2, \cdots$. Combining these local solutions over $[t_i, t_{i+1}]$ together, we could get a global approximate solution. Moreover, we can try to show this global approximate solution is bounded under some norm and its bound is independent of h. Finally, there is a subsequence of the global approximate solution converges to a global solution.

Remark 2.4.1: From **Remark 2.3.1**, **Remark 2.3.2** and Theorem $1-4$, it is not very difficult to see that the analyses and discussions of this section can be extended to the model with both diffusion and advection, such as (1.24).

Chapter 3

Computational Techniques for an Individual-Based Population Model

In this chapter, we will develop and analyze numerical schemes and computational strategy for the model of an individual-based fish population in a spatially heterogeneous chemical toxicant environment proposed in the previous chapters, which mainly consists of a mixed problem of an ordinary differential system and a partial differential problem. The ordinary differential system describes the individual model and the partial differential problem describes the individual-based population dynamics model. The general idea for the numerical scheme for the individual-based population model is to follow the three basic procedures of our mathematical analysis for the individual-based fish population mathematical model in last chapter, which are localization, unstructuralization of physiological variables and linearization. For the ordinary differential system of the individual model, we simply use the implicit Runge-Kutta method because of stiffness. However, it is much more complicated for the partial differential problem of the individual-based population dynamics since it is a nonlocal initial-boundary nonlinear partial differential problem with a discontinuous coefficient. In particular, it includes an integral equation (i.e., renewal equation) as a part of the initial-boundary conditions and its partial differential equation is indeed two equations unified by a discontinuous coefficient, one is quasi-linear hyperbolic and the other is nonlinear degenerate parabolic. To discretize the population dynamic model, we use a characteristic finite difference in the age-time domain and a finite element method with numerical integration in the spatial domain. As a preparation and basis to construct and analyze our numerical method for the individual-based population dynamics model, we construct and analyze the numerical schemes for the auxiliary age structured population dynamics models. Then, we discuss the computational model for the individual-based fish population model in a spatially heterogeneous chemical toxicant environment. The numerical schemes not only have optimal error estimates in the view point of numerical analysis but also always produce biologically reasonable approximate solutions.Finally, we discuss the computing and coding methodology for implementing the numerical scheme. As a very important related problem, we give a parallel procedure for solving large linear systems such as one obtained from our computational model, which is the core of the numerical implementation of the computational model.

3.1 Numerical Methods for Ordinary Differential Problems

As we have seen, there are ordinary differential system problems in the individual-based population models. Thus, to construct computational models for the individual-based population models, we first have to discuss numerical methods for ordinary differential problems. Because of stiffness (cf. [86, 90]), we need to apply an implicit Runge-Kutta method (cf. [76, 88]) to discretize the ordinary differential system problems.

Consider the following initial value problem of ordinary differential system:

$$\begin{aligned} \frac{dy}{dt} &= f(t,y), \qquad t \in (t_0, T], \\ y(t_0) &= y_0. \end{aligned} \tag{3.1}$$

We divide the interval $[t_0, T]$ into N small intervals $[t_i, t_{i+1}]$, where

$$\tau = \frac{T - t_0}{N}, \quad t_i = t_0 + i \cdot \tau, \quad i = 0, 1, \ldots, N.$$

The 1-stage implicit Runge-Kutta method for (3.1):

$$\begin{aligned} y_{i+1} &= y_i + f(t_i + \tfrac{1}{2}\tau, \tfrac{1}{2}(y_i + y_{i+1})), \quad i = 0, 1, \ldots, N \\ y_0 &= y(t_0). \end{aligned} \tag{3.2}$$

We have that from [76]

LEMMA 5 *The 1-stage implicit Runge-Kutta method* (3.2) *has the following error estimate:*

$$|y_i - y(t_i)| = O(\tau^2), \quad i = 1, 2, \ldots, N$$

where $y(t)$ *is the solution of* (3.1) *and* y_i *is defined in* (3.2).

In fact, the local truncation error can reach $O(\tau^3)$. Furthermore, when a higher error accuracy approximation is needed, we use the 2-stage implicit Runge-Kutta method as

$$\begin{aligned} y_{i+1} &= y_i + \frac{1}{2}\left[f(t_i + \frac{3+\sqrt{3}}{6}\tau, Y_1) + f(t_i + \frac{3-\sqrt{3}}{6}\tau, Y_2)\right] \\ &\qquad\qquad i = 0, 1, \ldots, N-1 \\ y_0 &= y(t_0) \end{aligned} \tag{3.3}$$

where

$$\begin{aligned} Y_1 &= y_i + \frac{3+\sqrt{3}}{6}\tau f(t_i + \frac{3+\sqrt{3}}{6}\tau, Y_1), \\ Y_2 &= \sqrt{3}y_i + (\sqrt{3}-1)Y_1 + \frac{3+\sqrt{3}}{6}\tau f(t_i + \frac{3-\sqrt{3}}{6}\tau, Y_2). \end{aligned} \tag{3.4}$$

Similarly, we have that (cf. [76])

LEMMA 6 *The 2-stage implicit Runge-Kutta method* (3.3) (3.4) *has the following error estimate:*

$$|y_i - y(t_i)| = O(\tau^3), \quad i = 1, 2, \cdots, N$$

where $y(t)$ *is the solution of* (3.1) *and* y_i *is defined in* (3.3) (3.4).

It is easy to see that we have to solve some nonlinear systems at each step when the function f in (3.1) is nonlinear. We usually use Newton's method to solve nonlinear systems. To describe Newton's method, we rewrite nonlinear systems as following general form: find $x \in \mathcal{R}^n$ such that

$$F(x) = 0, \tag{3.5}$$

where $F : \mathcal{R}^n \longrightarrow \mathcal{R}^n$, a continuously differential mapping. Then, Newton's method for solving (3.5) is (cf. [57]).

$$\begin{aligned} J(x_i)s_i &= -F(x_i), \\ x_{i+1} &= x_i + s_i, \\ & \quad i = 1, 2, \cdots \end{aligned} \tag{3.6}$$

where $x_0 \in \mathcal{R}^n$ is a given initial guess, J is the Jacobi matrix. It is well-known that Newton's method (3.6) has a quadratic convergence if x_0 is chosen properly. However, if F is not continuously differentiable or the Jacobian J is not easily computed, we will use the following Broyden's method (cf. [57]).

$$\begin{aligned} A_i s_i &= -F(x_i), \\ x_{i+1} &= x_i + s_i, \\ y_i &= F(x_{i+1}) - F(x_i), \\ A_{i+1} &= A_i + \frac{(y_i - A_i s_i)s_i^T}{s_i^T s_i}, \\ & \quad i = 1, 2, \cdots \end{aligned} \tag{3.7}$$

where $x_0 \in \mathcal{R}^n$ and $A_0 \in \mathcal{R}^{n \times n}$ are given initial values. Broyden's method has a super-linear convergence if x_0 and A_0 is chosen properly.

3.2 Numerical Schemes for Population Models

To build computational models for the individual-based fish population models proposed in the previous chapters, we first need to design and analyze numerical schemes for three auxiliary age structured population mathematical models of Chapter 2. We consider the time domain (interval) $(0, T]$ and age domain (interval) $[0, A_m]$, where A_m is the maximum age of the fish. In order to construct characteristic time-age finite difference schemes (cf. [14, 65, 86, 88, 98, 98, 108]), we have to choose the same step size, say τ, to partition both $(0, T]$ and $[0, A_m]$

as follows:

$$\begin{aligned} 0 &= t_0 < t_1 < t_2 < \ldots < t_{N_t} = T, \\ 0 &= a_0 < a_1 < a_2 < \ldots < a_{N_a} = A_m, \end{aligned} \tag{3.8}$$

where

$$\begin{aligned} t_i &= t_0 + i \cdot \tau = t_0 + i \cdot \frac{T - t_0}{N_t}, \quad i = 1, 2, \cdots, N_t \\ a_i &= a_0 + i \cdot \tau = a_0 + i \cdot \frac{A_m}{N_a}, \quad i = 1, 2, \cdots, N_a. \end{aligned} \tag{3.9}$$

We also consider the spatial domain $\Omega \subset \mathcal{R}^{\mathrm{n}}$ ($\mathbf{n} = 1,\ 2,\ 3$), a bounded open set with a suitably smooth boundary $\partial\Omega$. To construct finite element approximations on the spatial domain Ω (cf. [15, 25, 63, 64, 107]), we introduce a finite element triangulation $\mathcal{J}_h$ for Ω. We assume that $\mathcal{J}_h$ is a regular and quasi-uniform simplex partition of Ω with mesh size h. Roughly speaking, we partition Ω into simplexes with edge length $O(h)$. For simplicity, we also assume that $\bar{\Omega} = \bigcup_{e \in \mathcal{J}_h} \bar{e}$, where e is an element (*small simplex*) of $\mathcal{J}_h$.

These same notations are applied in the remainder of this Chapter. Also, we assume that C is a generic constant in the remainder of the thesis, which may be a different value while appearing in different locations, however, it is always independent of τ and h and only dependent of the related given data.

3.2.1 Numerical Scheme for Age structured Population Problem (I)

This subsection is to consider the age structured population problem (I) defined by (2.5) in last chapter. We have developed and analyzed a numerical scheme to discretize this problem. For convenience, we rewrite the problem here.

$$\begin{aligned} \frac{\partial u}{\partial t} + \frac{\partial u}{\partial a} &= -\mu u \\ u(0,a) &= u_0(a) \\ u(t,0) &= \int_0^{A_m} \beta u(t,a)\, da \end{aligned} \tag{3.10}$$

where $\mu = \mu(t,a,P)$, $\beta = \beta(t,a,P)$, and

$$P \equiv P(t) = \int_0^{A_m} u(t,a)\, da.$$

The finite difference approximations for (3.10) have been discussed by several researchers (cf. [14, 61, 65, 74]). Moreover, our numerical scheme can be regarded as modifications of their schemes since we always assume that fish have a finite maximum age. It is clearly natural to apply a characteristic finite difference method to discretize (3.10) because of the natural relationship between age and time. Notice that

$$\lim_{\tau \to 0} \frac{u(t+\tau, a+\tau) - u(t,a)}{\tau} = \frac{\partial u}{\partial t} + \frac{\partial u}{\partial a} \equiv \partial_\tau u$$

we then can apply the following characteristic finite difference approximation in the numerical scheme

$$\bar{\partial}_\tau u^{n,j} \equiv \frac{u^{n,j} - u^{n-1,j-1}}{\tau} \approx (\frac{\partial u}{\partial t} + \frac{\partial u}{\partial a})|_{(t_n,a_j)} \equiv \partial_\tau u|_{(t_n,a_j)} \tag{3.11}$$

where $u^{n,j}$ stands for an approximation of $u(t_n, a_j)$. Thus, we can construct the following time-age characteristic finite difference method for (3.10):

$$\begin{aligned} \frac{u^{n,j} - u^{n-1,j-1}}{\tau} &= -\tilde{\mu}^{n-1,j} u^{n,j}, \\ & \qquad j = 1, 2, \ldots, N_a, \quad n = 1, 2, \ldots, N_t \\ u^{0,j} &= u_0(a_j) \\ u^{n,0} &= \frac{1}{2}\tilde{\beta}^{n-1,0} u^{n,0}\tau + \sum_{j=1}^{j=N_a} \tilde{\beta}^{n-1,j} u^{n,j}\tau \\ P^n &= \frac{1}{2} u^{n,0}\tau + \sum_{j=0}^{j=N_a} u^{n,j}\tau \end{aligned} \tag{3.12}$$

where $\tilde{\mu}^{n-1,j}$ and $\tilde{\beta}^{n-1,j}$ are approximate values for $\mu(t_n, a_j, P(t_n))$ and $\beta(t_n, a_j, P(t_n))$, respectively, which are defined by the technique of involving a delay τ as follows.

$$\begin{aligned} \tilde{\mu}^{n-1,j} &= \mu(t_n, a_j, P^{n-1}) \\ \tilde{\beta}^{n-1,j} &= \beta(t_n, a_j, P^{n-1}). \end{aligned}$$

In addition, the solution of (3.10) always satisfies $u(t, A_m) = 0$ since A_m is the maximum age; we then assume explicitly here that

$$u^{n,N_a} = 0, \quad n = 1, 2, \cdots, N_t. \tag{3.13}$$

It is not hard to see that the numerical scheme (3.12) is linear. Furthermore, we have the following two lemmas for the bound and error estimates for the numerical scheme (3.12)–(3.13).

LEMMA 7 *Assume that* u_0*,* μ *and* β *are all nonnegative continuous functions over their own variable domain and* β *satisfies*

$$0 \leq \beta \leq \bar{\beta} < \infty.$$

Then, if τ *is sufficiently small, there exists a generic constant* C*, independent of* τ*, such that, for* $j = 0, 1, \cdots, N_a$ *,* $n = 1, 2, \cdots, N_t$*,*

$$0 \leq u^{n,j} \leq C$$
$$0 \leq P^n \leq C.$$

where $u^{n,j}$ *and* P^n *are defined in* (3.12).

Proof. Notice that $\mu \geq 0$ and (3.12), it is easy to see that, for $j = 0, 1, \cdots, N_a$,

$n = 1, 2, \cdots, N_t$,

$$u^{n,j} \geq 0, \qquad P^n \geq 0. \tag{3.14}$$

Multiplying the first equality of (3.12) with τ^2 and summing it over $1 \leq j \leq N_a$, then, from (3.12) - (3.13), we have that

$$P^n = P^{n-1} + \frac{1}{2}\tau u^{n,0} - \frac{1}{2}\tau u^{n-1,0} - \tau \sum_{j=0}^{j=N_a} \tilde{\mu}^{n-1,j} u^{n,j} \tau$$

$$u^{n,0} \leq \frac{1}{2}\bar{\beta} u^{n,0}\tau + \bar{\beta} \sum_{j=1}^{j=N_a} u^{n,j}\tau = \bar{\beta} P^n. \tag{3.15}$$

Therefore,

$$\begin{aligned} P^n &\leq P^{n-1} + \frac{1}{2}\tau u^{n,0} \\ &\leq P^{n-1} + \frac{1}{2}\tau \left(\frac{1}{2}\tilde{\beta}^{n-1,0} u^{n,0}\tau + \sum_{j=1}^{j=N_a} \tilde{\beta}^{n-1,j} u^{n,j}\tau \right) \\ &\leq P^{n-1} + \frac{1}{2}\bar{\beta}\,\tau\, P^n. \end{aligned}$$

Thus, if τ is sufficiently small such that

$$1 - \bar{\beta}\tau > 0,$$

then we have

$$P^n \leq \frac{P^{n-1}}{1-\frac{1}{2}\tau\bar{\beta}} \leq (1+\tau\bar{\beta})\,P^{n-1}.$$

So,

$$P^n \leq (1+\tau\bar{\beta})^n P^0.$$

which implies that, for $n = 1, 2, \cdots, N_t$,

$$P^n \leq P^0 \exp(\bar{\beta}T) \leq C. \tag{3.16}$$

By the first equality of (3.12), (3.14) and (3.15),

$$u^{n,j} \leq \begin{cases} u^{0,j-n} = u_0(a_{j-n}) \leq C, & \text{if } j \geq n \\ u^{n-j,0} \leq \bar{\beta}P^{n-j} \leq C, & \text{if } j < n. \end{cases}$$

Hence, which, together with (3.14) and (3.16), clearly imply the results of Lemma 7. Thus, we have completed the proof.

LEMMA 8 *Assume that all the assumptions of Lemma 7 hold and* μ *has bounded first derivatives with respect to all of its own variables over* $[0,t]\times[0,A_m)\times(0,+\infty)$. *Then we have the following error estimates, for* $j = 0, 1, \cdots, N_a, n = 1, 2, \cdots, N_t$,

$$|u(t_n, a_j) - u^{n,j}| \leq C\tau$$

$$|P(t_n) - P^n| \leq C\tau$$

where C is a generic constant, independent of τ.

Proof. For convenience, we denote by

$$\begin{aligned}
\xi^{n,j} &= u(t_n, a_j) - u^{n,j}, \ \ j = 0, 1, \cdots, N_a - 1, \ n = 0, 1, \cdots, N_t \\
\zeta^n &= P(t_n) - P^n, \quad n = 0, 1, \cdots, N_t \\
\xi^n &= (\xi^{n,0}, \xi^{n,1}, \cdots, \xi^{n,N_a}), \quad n = 0, 1, \cdots, N_t \\
\|\xi^n\|_{\ell^1} &= \sum_{j=0}^{N_a} | \, \xi^{n,j} \, |, \quad n = 0, 1, \cdots, N_t.
\end{aligned}$$

Therefore, from (3.10) and (3.12),

$$\begin{aligned}
&\frac{\xi^{n,j} - \xi^{n-1,j-1}}{\tau} \\
&= \frac{u(t_n, a_j) - u(t_{n-1}, a_{j-1})}{\tau} - \frac{u^{n,j} - u^{n-1,j-1}}{\tau} \\
&= -\mu(t_n, a_j, P(t_n))u(t_n, a_j) + \tilde{\mu}^{n-1,j} u^{n,j} + O(\tau) \\
&= -\tilde{\mu}^{n-1,j} \xi^{n,j} + (\tilde{\mu}^{n-1,j} - \mu(t_n, a_j, P(t_n)) \,) \, u(t_n, a_j) + O(\tau).
\end{aligned}$$

By the mean value theorem for μ, there exists a p, whose value is between $P(t_n)$ and P^{n-1}, such that

$$\begin{aligned}
\tilde{\mu}^{n-1,j} - \mu(t_n, a_j, P(t_n) &= \mu(t_n, a_j, P^{n-1}) - \mu(t_n, a_j, P(t_n) \\
&= \frac{\partial \mu}{\partial P}\Big|_{(t_n, a_j, p)} \, (P^{n-1} - P(t_n) \,) \\
&= C\zeta^{n-1} + O(\tau).
\end{aligned}$$

Then, from Lemma 7, we have that

$$\frac{\xi^{n,j} - \xi^{n-1,j-1}}{\tau} = -\tilde{\mu}^{n-1,j}\,\xi^{n,j} + C|\zeta^{n-1}| + O(\tau),$$

that is,

$$(1 + \tau\tilde{\mu}^{n-1,j})|\xi^{n,j}| \leq |\xi^{n-1,j-1}| + C\tau|\zeta^{n-1}| + O(\tau^2). \tag{3.17}$$

Furthermore, it follows from the trapezoidal rule,

$$\begin{aligned} |\zeta^n| &= \left| \int_0^{A_m} u(t_n, a)da - (\frac{1}{2}u^{n,0}\tau + \sum_{j=1}^{N_a} u^{n,j}\tau) \right| \\ &\leq \|\xi^n\|_{\ell^1} + O(\tau). \end{aligned} \tag{3.18}$$

Therefore, which, together with (3.17), implies

$$|\xi^{n,j}| \leq |\xi^{n-1,j-1}| + C\tau\|\xi^{n-1}\|_{\ell^1} + C\tau^2. \tag{3.19}$$

Multiplying (3.19) by τ and summing it form $j = 1$ to $j = N_a$, we then obtain that

$$\|\xi^n\|_{\ell^1} - \tau|\xi^{n,0}| \leq (1 + C\tau)\|\xi^{n-1}\|_{\ell^1} + C\tau^2.$$

It follows from Lemma 7 and the trapezoidal rule that

$$
\begin{aligned}
|\xi^{n,0}| &= \left| \int_0^{A_m} \beta(t_n a, P(t_n))\, u(t_n, a)\, da - (\frac{1}{2}\tilde{\beta}^{n-1,0} u^{n,0} \tau + \sum_{j=1}^{N_a} \tilde{\beta}^{n-1,j} u^{n,j} \tau) \right| \\
&\leq \frac{1}{2}\bar{\beta}^{n-1,0} \xi^{n,0} \tau + \bar{\beta} \sum_{j=1}^{N_a} |\xi^{n,j}| \tau + C|\zeta^{n-1}| + O(\tau) \\
&\leq \bar{\beta} \|\xi^n\|_{\ell^1} + C\|\xi^{n-1}\|_{\ell^1} + O(\tau).
\end{aligned}
$$

Then we have

$$(1 - \tau\bar{\beta})\|\xi^n\|_{\ell^1} \leq (1 + C\tau)\|\xi^{n-1}\|_{\ell^1} + C\tau^2.$$

Noting that

$$\xi^{0,j} = 0, \quad j = 0, 1, \cdots, N_a \tag{3.20}$$

and using Gronwall's inequality we have that, if τ is sufficiently small, then

$$\|\xi^n\|_{\ell^1} \leq C\,\tau \qquad n = 1, 2, \cdots, N_t. \tag{3.21}$$

Hence, combining all formulations from (3.18) to (3.21) together, we have that

$$|\zeta^n| \ = \ |P(t_n) - P^n| \leq C\tau,$$

and

$$\begin{aligned} |\xi^{n,0}| &\leq C\tau, \\ |\xi^{n,j}| &\leq |\xi^{n-1,j-1}| + C\tau^2. \end{aligned} \tag{3.22}$$

Thus, we finally have that from (3.20) and (3.22)

$$\begin{aligned} |\xi^{n,j}| &= |u(t_n, a_j) - u^{n,j}| \\ &\leq \begin{cases} |\xi^{0,j-n}| + C\tau \leq C\tau, & \text{if } j \geq n \\ |\xi^{n-j,0}| + C\tau \leq C\tau, & \text{if } j < n. \end{cases} \end{aligned}$$

Clearly, we have completed the proof.

Remark 3.2.1.1: From the definition of local truncation error, we have from the second inequality of (3.22) that the numerical scheme (3.12) has an $O(\tau^2)$ local truncation error estimate.

Remark 3.2.1.2: If we choose an approximate value of $u^{0,j}$ instead of the exact initial value $u^{0,j}$ such that $u^{0,j}$ satisfies: $|\xi^{0,j}| = |u(0, a_j) - u^{0,j}| = O(\tau^2)$, we then have from the proofs that Lemma 7, Lemma 8 and **Remark 3.2.1.1** are still true.

3.2.2 Numerical Scheme for Age structured Population Problem (II)

This subsection considers the second auxiliary age structured population problem (II) defined in Section 2.3 of Chapter 2, which is a nonlocal initial-boundary nonlinear degenerate parabolic partial differential problem. We have developed and analyzed a numerical scheme to discretize this problem. The basic idea to construct the numerical scheme is to use a characteristic finite difference discretization for the time-age domain and a finite element discretization with numerical integral modification for the spatial domain. We have shown that the numerical scheme not only has the optimal convergence error estimate but also ensures that a biologically valid approximate solution is obtained.

For convenience, we rewrite the problem the auxiliary age structured population problem (II) as follows.

$$\begin{aligned}
&\frac{\partial u}{\partial t}+\frac{\partial u}{\partial a}-\nabla\cdot(k\nabla u)=-\mu u,\\
&\qquad\qquad t\in(0,T],\ a\in[0,A_m],\ x\in\Omega\\
&k\frac{\partial u}{\partial \nu}=0 \quad or \quad u=0, \quad \text{on} \quad \partial\Omega\\
&u(0,a,x)=u_0(a,x)\\
&u(t,0,x)=\int_0^{A_m}\beta u(t,a,x)da
\end{aligned} \tag{3.23}$$

where $k=k(t,x,P)$, $\mu=\mu(t,a,x,P)$, $\beta=\beta(t,a,x,P)$, and

$$P\equiv P(t,x)=\int_0^{A_m}u(t,a,x)da.$$

We also recall its weak formulation: find $u : (0, T] \times [0, A_m] \longrightarrow V$, such that

$$\begin{aligned}
&(\partial_\tau u,\ w) + \alpha(k,\ u,\ w) = -(\mu\, u,\ w), \qquad \forall\, w \in V \\
&u(0, a, x) = u_0(a, x) \\
&u(t, 0, x) = \int_0^{A_m} \beta u(t, a, x) da
\end{aligned} \tag{3.24}$$

where the notations are previously defined, in particular,

$$\partial_\tau u = \frac{\partial u}{\partial t} + \frac{\partial u}{\partial a} \tag{3.25}$$

$$\alpha(k,\ v,\ w) = (k\, \nabla u,\ \nabla w) = \int_\Omega k \nabla u \cdot \nabla w dx. \tag{3.26}$$

We have discussed some mathematical analyses for (3.24) in Chapter 2. We now develop a numerical discretization for (3.24). The finite element and finite difference numerical approximations for (3.24) and some of its similar related problems in 1-*dimensional* and 2-*dimensional* domains have been considered (cf. [64, 86, 91]). Our numerical scheme is close to that in [64], however, since the special numerical quadratures and other numerical techniques, such as the upwind finite element technique and upwind finite difference technique, have been applied in the scheme, the numerical schemes not only have optimal error estimates in the view point of numerical analysis but also always produce biologically reasonable approximate solutions. Furthermore, our numerical analysis method also has some difference from that in [64] because of the difference of the schemes. We use the partition defined in (3.8) (3.9) to discretize the time-age domain $[0, t] \times [0, A_m]$, whose step (mesh) size is τ, and the finite element triangulation $\mathcal{J}_h$ defined at the beginning of this section to partition the spatial domain Ω, whose mesh size is h. Let $V_h \subset (C^0(\bar{\Omega}) \cap V)$ be the linear conforming triangle finite element approximation space to V over the triangulation $\mathcal{J}_h$. For detailed definition of V_h, we refer to [15, 22, 63, 107]. Thus, we can introduce the characteristic finite difference – finite element numerical approximation scheme with numerical integration for (3.24) as follows: find $u_h^{n,j} \in V_h$, such that

$$\begin{aligned}
&(\tilde{\partial}_\tau u_h^{n,j},\ w)_h + \alpha_h(\tilde{k}_h^{n-1},\ u_h^{n,j},\ w) = -(\tilde{\mu}_h^{n-1,j}\, u_h^{n,j},\ w)_h, \\
&\qquad\qquad \forall\, w \in V_h\,,\ j = 1, \cdots, Na, \quad n = 1, 2, \cdots, N_t \\
&u_h^{0,j} = \pi_h(\, u(a_j, x)\,), \quad \forall\, j = 0, 1, \cdots, N_a \\
&P_h^0 = \frac{1}{2} u_h^{0,0} \tau + \sum_{j=1}^{Na-1} u_h^{0,j} \tau \\
&u_h^{n,0} = \frac{1}{2} \tilde{\beta}_h^{n-1,0} u_h^{n,0} \tau + \sum_{j=1}^{Na-1} \tilde{\beta}_h^{n-1,j} u_h^{n,j} \tau \\
&P_h^n = \frac{1}{2} u_h^{n,0} \tau + \sum_{j=1}^{Na-1} u_h^{n,j} \tau, \quad \forall\, 1 \le n \le N_t
\end{aligned} \tag{3.27}$$

where $\alpha_h(\cdot,\cdot,\cdot)$ is an approximation of $\alpha(\cdot,\cdot,\cdot)$ defined in (3.26) by using a technique of numerical integration, $(\cdot,\cdot)_h$ is an approximation of the L^2-inner product $(\cdot,\cdot)$ over Ω by a technique of numerical integration, too, π_h is a linear operator for V to V_h, and

$$\begin{aligned}
\tilde{\partial}_\tau u_h^{n,j} &= \frac{u_h^{n,j} - u_h^{n-1,j-1}}{\tau} \\
\tilde{k}_h^{n-1} &= k(t_n, x, P_h^{n-1}) \\
\tilde{\mu}_h^{n-1,j} &= \mu(t_n, a_j, x, P_h^{n-1}) \\
\tilde{\beta}_h^{n-1,j} &= \beta(t_n, a_j, x, P_h^{n-1}).
\end{aligned} \tag{3.28}$$

Clearly, while choosing the approximate values $\tilde{k}_h^{n-1}$, $\tilde{\mu}_h^{n-1,j}$ and $\tilde{\beta}_h^{n-1,j}$, we have used the technique involving a delay τ. In addition, since the solution $u(t,a,x)$ of (3.24) satisfies $u(t, A_m, x) = 0$, we explicitly assume that

$$u_h^{n,N_a} = 0, \quad \text{on } \Omega, \quad n = 1, 2, \cdots, N_t. \tag{3.29}$$

Denote by $b_{e,j}$ a vertex of $e \in \mathcal{J}_h$. We now give the definition of $(\cdot,\cdot)_h$, $\alpha_h(\cdot,\cdot,\cdot)$ and π_h. Noting that $\Omega \subset \mathcal{R}^{\mathbf{n}}$, a $\mathbf{n}$-dimensional domain, we then define

$$\begin{aligned}
(\psi\, v,\ w)_h &= \sum_{e \in \mathcal{J}_h} \frac{1}{\mathbf{n}+1} meas(e) \sum_{b_{e,j}} (\psi\, v\, w)(b_{e,j}) \\
\alpha_h(k, v, w) &= (k\, \nabla v,\ \nabla w)_h \\
&= \sum_{e \in \mathcal{J}_h} \frac{1}{\mathbf{n}+1} meas(e) \sum_{b_{e,j}} k((b_{e,j}) \nabla v|_e \cdot \nabla w|_e
\end{aligned}$$

where $meas(\cdot)$ stands for a $\mathbf{n}$-*dimensional* measurement. The linear operator $\pi_h : V \longrightarrow V_h$ is either the standard linear conforming triangle finite element interpolation operator (cf. [15, 63])

$$\pi_h v(b_{e,j}) = v(b_{e,j}), \quad \text{for} \quad \forall\, e \in \mathcal{J}_h$$

or the standard H^1-project operator as follows (cf. [15, 63])

$$(\nabla(v - \pi_h v), \nabla w) + (v - \pi_h v, w) = 0\,, \quad \text{for } \forall\, w \in V_h.$$

Moreover, for both definitions of π_h, we have the following properties.

$$\begin{aligned} &\|v - \pi_h v\|_0 + h\|\nabla(v - \pi_h v)\|_0 \le Ch^2\|v\|_2 \\ &\|\pi_h v\|_{0,\infty} + |\pi_h v|_{1,\infty} \le C\min(\|v\|_{C^1}, \|v\|_{2,\infty}) \end{aligned} \tag{3.30}$$

as in last chapter, where $\|\cdot\|_m$ ($|\cdot|_m$) and $\|\cdot\|_{m,p}$ ($|\cdot|_{m,p}$) are the standard norm (semi-norm) of Sobolev spaces $H^m(\Omega)$ and $W^{m,p}(\Omega)$, respectively (cf. [1, 34, 63]).

Furthermore, let $\mathcal{N}_h$ be the *true* unknown node point set of V_h and let $\{\varphi_i\}_{i\in\mathcal{N}_h}$ be the standard finite element basis functions of V_h (cf. [15, 60, 63]). Then $u_h^{n,j}$ in (3.27) may be expressed as

$$u_h^{n,j} = \sum_{i\in\mathcal{N}_h} U_i^{n,j}\varphi_i, \quad U^{n,j} = (U_i^{n,j})_{i\in\mathcal{N}_h}, \quad U_i^{n,j} \in \mathcal{R}. \tag{3.31}$$

Therefore, plugging (3.31) into the approximate problem (3.27), the first equality, which is the core portion of the approximate problem (3.27), can be rewritten as the following linear system, which includes $|\mathcal{N}_h|$, the cardinal number of $\mathcal{N}_h$, unknowns

$$\left(\frac{1}{\tau}M + A + D\right) U^{n,j} = \frac{1}{\tau}M\, U^{n-1,j-1} \tag{3.32}$$

where

$$\begin{aligned} M &= (m_{rs})_{|\mathcal{N}_h|\times|\mathcal{N}_h|}, \quad m_{rs} = (\varphi_r, \varphi_s)_h \\ A &= (\alpha_{rs})_{|\mathcal{N}_h|\times|\mathcal{N}_h|}, \quad \alpha_{rs} = \alpha_h(\tilde{k}_h^{n-1}, \varphi_r, \varphi_s) \\ D &= (d_{rs})_{|\mathcal{N}_h|\times|\mathcal{N}_h|}, \quad d_{rs} = (\tilde{\mu}_h^{n-1,j}\varphi_r, \varphi_s)_h. \end{aligned} \tag{3.33}$$

It is easy to see that solving the linear system (3.32) is a very large part of problem (3.27) at each step. In particular, for high dimension problems, it is a very important issue how to solve the linear system (3.32) since it is ill-conditioned. We will give a parallel method to solve (3.32) sufficiently later.

To ensure obtain a good biologically approximate solution, we assume that $\mathcal{J}_h$ is *weakly acute* (cf. [16, 59, 100]), that is, for the standard basis functions $\{\varphi_i\}_{i\in\mathcal{N}_h}$

$$\int_\Omega \nabla\varphi_i \cdot \nabla\varphi_j \, dx \leq 0, \qquad \text{for } \; i \neq j, \; i,j = 1, 2, \cdots, |\mathcal{N}_h|. \tag{3.34}$$

Clearly, $\mathcal{J}_h$ is always weakly acute for a 1-*dimension* domain Ω. For a 2-*dimension* domain Ω, that every triangle in $\mathcal{J}_h$ is not obtuse is a sufficient condition to show that $\mathcal{J}_h$ is weakly acute (cf. [16, 100]). But it is very complicated for a 3-*dimension* domain. We now have several mesh generator software packages to partition a weakly acute mesh automatically (cf. [97]). We also assume $\tau = O(h^2)$, in particular, $O(h^2) \leq \tau \leq O(h)$ such that we can get a good convergence error estimate for the approximation solutions (cf. [88, 107, 108]).

THEOREM 5 *Let* k *be a continuous function satisfying*

$$k_2 \geq k = k(t,a,x,P) \geq k_1 > 0, \quad \text{on} \ \ [0,T] \times [0,A_m] \times \Omega \times (0,+\infty), \tag{3.35}$$

μ *be a continuous function satisfying*

$$0 \not\equiv \mu = \mu(t,a,x,P) \geq \bar{\mu}, \quad \text{on} \ \ [0,T] \times [0,A_m) \times \Omega \times (0,+\infty), \tag{3.36}$$

and β *be a continuous function satisfying*

$$\bar{\beta} \geq \beta = \beta(t,a,x,P) \geq 0, \quad \text{on} \ \ [0,T] \times [0,A_m] \times \Omega \times (0,+\infty), \tag{3.37}$$

where k_1, k_2, $\bar{\mu}$ *and* $\bar{\beta}$ *are constants. Also, let* $u_0 \in V \cap C(\Omega)$ *be nonnegative. Then, the numerical approximate problem* (3.27) *has a unique nonnegative solution.*

Proof. Notice that from (3.27) and (3.32), it is sufficient to show that, for any $j = 1, 2, \cdots, N_a - 1$ and $n = 1, 2, \cdots, N_t$, the linear system (3.32) has a unique solution $U^{n,j}$ satisfying

$$U^{n,j} \geq 0, \quad \text{if} \ \ U^{n-1,j-1} \geq 0 \tag{3.38}$$

where $U^{r,s} \geq 0$ means each of its component is nonnegative ($r = n, n-1,\ s = j, j-1$).

It is easy to show that

$$B = \frac{1}{\tau}M + A + D$$

is a $|\mathcal{N}_h| \times |\mathcal{N}_h|$ symmetric positive matrix. This clearly implies that (3.32) has a unique solution $U^{n,j}$.

On the other hand, from [3, 16, 30, 36, 110], both M and D are positive definite diagonal matrices. Also, since $\mathcal{J}_h$ is weakly acute, (3.34) implies that A has positive diagonal elements and non positive off-diagonal elements. So, the coefficient matrix of (3.32), $B = \frac{1}{\tau}M + A + D$, is a *M-Matrix* (cf. [3, 30, 110]). Therefore, in view of [3, 36, 110], this implies (3.38). We thus complete the proof.

Denote by

$$||v||_h = (v, v)_h, \quad \text{for } \forall \quad v \in V_h. \tag{3.39}$$

It is easy to check that $|| \cdot ||_h$ is uniformly equivalent to the standard $L^2 - norm$ $|| \cdot ||_0$, in fact, we have that (cf. [35, 63, 106])

$$\frac{1}{2}||v||_0 \leq ||v||_h \leq 2||v||_0, \quad \text{for } \forall \quad v \in V_h. \tag{3.40}$$

We then have that

THEOREM 6 *Assume that all assumptions of Theorem* 5 *hold. Let* $u_h^{n,j}$ *and* P_h^n *be defined by the numerical approximate problem* (3.27). *Then, there exist a constant* C*, independent of* h *and* τ*, such that*

$$\begin{aligned} \|u_h^{n,j}\|_0 &\leq C, \quad j=0,1,\cdots,N_a,\ n=1,2,\cdots,N_t \\ \|P_h^n\|_0 &\leq C, \quad n=1,2,\cdots,N_t. \end{aligned}$$

Proof. Taking $w=u_h^{n,j}$ in the first equality of (3.27), we have

$$\frac{1}{\tau}(u_h^{n,j}-u_h^{n-1,j-1},u_h^{n,j})_h+\alpha_h(\tilde{k}_h^{n-1},u_h^{n,j},u_h^{n,j})=-(\tilde{\mu}_h^{n-1,j}u_h^{n,j},u_h^{n,j})_h.$$

Hence,

$$(u_h^{n,j},u_h^{n,j})_h\leq(u_h^{n-1,j-1},u_h^{n,j})_h. \tag{3.41}$$

By Schwartz inequality,

$$\|u_h^{n,j}\|_h\leq\|u_h^{n-1,j-1}\|_h.$$

Therefore,

$$\|u_h^{n,j}\|_h\leq\begin{cases}\|u_h^{0,j-n}\|_h, & \text{if } j\geq n\\ \|u_h^{n-j,0}\|_h, & \text{if } j<n.\end{cases} \tag{3.42}$$

If $j \geq n$, it follows from (3.27) and (3.30) that

$$\|u_h^{0,j-n}\|_h = \|\pi_h u_0\|_h \leq C. \tag{3.43}$$

On the other hand, if $j < n$, from (3.27) and (3.28)

$$\begin{aligned} \|u_h^{n-j,0}\|_h &= \|\frac{1}{2}\tilde{\beta}_h^{n-j-1,0} u_h^{n-j,0} \tau + \sum_{m=1}^{N_a} \tilde{\beta}_h^{n-j,m} u_h^{n-j,m} \tau\|_h \\ &\leq \bar{\beta}\|P_h^{n-j}\|_h. \end{aligned} \tag{3.44}$$

Multiplying (3.41) by τ and summing over $j = 0$ to N_a, we get

$$(P_h^n - \frac{1}{2}\tau\tilde{\beta}^{n-1,0} u_h^{n,0}, u_h^{n,j})_h \leq (P_h^{n-1} + \frac{1}{2}\tau\tilde{\beta}^{n-2,0} u_h^{n-1,0}, u_h^{n,j})_h.$$

Again, multiplying by τ, summing over $j = 0$ to N_a and by Schwartz inequality, we have that

$$\|P_h^n - \frac{1}{2}\tau\tilde{\beta}^{n-1,0} u_h^{n,0}\|_h \leq \|P_h^{n-1} + \frac{1}{2}\tau\tilde{\beta}^{n-2,0} u_h^{n-1,0}\|_h.$$

Notice that the results of Theorem 5 and the assumptions of this Theorem, we have that from (3.27)

$$\begin{aligned} (1 - \frac{1}{2}\tau\bar{\beta})\|P_h^n\|_h &\leq \|P_h^n - \frac{1}{2}\tau\bar{\beta}P_h^n\|_h \\ &\leq \|P_h^n - \frac{1}{2}(\frac{1}{2}\tau\tilde{\beta}_h^{n-1,0} u_h^{n,0} + \sum_{m=1}^{N_a} \tau\tilde{\beta}_h^{n-1,m} u_h^{n,m})\tau\|_h \end{aligned}$$

$$
\begin{aligned}
&\leq \|P_h^n - \frac{1}{2}\tau\tilde{\beta}^{n-1,0}u_h^{n,0}\|_h \\
&\leq \|P_h^{n-1} + \frac{1}{2}\tau\tilde{\beta}^{n-2,0}u_h^{n-1,0}\|_h \\
&\leq (1+\frac{1}{2}\tau\bar{\beta})\|P_h^{n-1}\|_h,
\end{aligned}
$$

which implies that

$$
\|P_h^n\|_h \leq \frac{1+\frac{1}{2}\tau\bar{\beta}}{1-\frac{1}{2}\tau\bar{\beta}}\|P_h^{n-1}\|_h \leq \left(\frac{1+\frac{1}{2}\tau\bar{\beta}}{1-\frac{1}{2}\tau\bar{\beta}}\right)^n \|P_h^0\|_h.
$$

This, together with (3.42) – (3.44), implies that, for $j = 0, 1, \cdots, N_a$, $n = 1, 2, \cdots, N_t$,

$$
\|P_h^n\|_h \leq C, \quad \|u_h^{n,j}\|_h \leq C.
$$

Finally, this together with (3.40) has completed the proof.

We now consider the convergence error estimates for the numerical approximate scheme defined in (3.27). Before estimating the error, we need to introduce some auxiliary lemmas and results about the corresponding auxiliary elliptic problem of (3.23).We consider the following auxiliary elliptic problem:

$$
\begin{aligned}
&-\nabla\left(k\nabla\Phi\right) + \mu\,\Phi = g \quad \text{on } \Omega \\
&k\frac{\partial\Phi}{\partial\nu} = 0 \;\text{ or }\; \Phi = 0 \quad \text{on } \partial\Omega
\end{aligned}
\tag{3.45}
$$

its variational formulation is: find $u \in V$ such that

$$\alpha(k,\, w,\, \Phi) + (\mu\, w,\, \Phi) = (w,\, g) \qquad \forall\, w \in V. \tag{3.46}$$

By the fundamental theory of partial differential problems (cf. [34, 63, 84]), if Ω is smooth enough, there then exists a unique solution $\Phi \in V$ to satisfy (3.46). Moreover, we have that $\Phi \in H^2(\Omega) \cap V$ and the following prior estimate

$$\|\Phi\|_2 \leq C\|g\|_0. \tag{3.47}$$

We are not going to discuss the existence and prior estimates of (3.45). We refer readers to find them from [34, 66, 84]. However, here and hereafter we will assume that (3.46) has a unique solution satisfying (3.47). We also introduce two elliptic projection operators: $\Lambda_h : \ v \in V \longrightarrow \ \Lambda_h v \in V_h,$ determined by

$$\alpha(k, v - \Lambda_h v,\, w) + (\mu\,(v - \Lambda_h v),\, w) = 0, \quad \forall\, w \in V \tag{3.48}$$

and $\tilde{\Lambda}_h : \ v \in V \longrightarrow \ \tilde{\Lambda}_h v \in V_h$ determined by

$$\alpha_h(k, \tilde{\Lambda}_h v,\, w) + (\mu\, \tilde{\Lambda}_h v, w)_h = \alpha(k,\, v,\, w) + (\mu\, v, w), \quad \forall\, w \in V. \tag{3.49}$$

It is not hard to confirm that Λ_h and $\tilde{\Lambda}_h$ are well-defined. Moreover, we have

LEMMA 9 *Assume that all assumptions of Theorem* 5 *hold and* k *has bounded first derivatives with respect to all of its variables. Then we have*

$$\begin{aligned} \|v-\Lambda_h v\|_0 + h\|v-\Lambda_h v\|_1 &\leq Ch^2\|v\|_2 \quad \forall\, v \in H^2(\Omega)\cap V \\ \|v-\tilde{\Lambda}_h v\|_0 + h\|v-\tilde{\Lambda}_h v\|_1 &\leq Ch^2\|v\|_2, \quad \forall\, v \in H^2(\Omega)\cap V \end{aligned}$$

where the constant C *is dependent of* k *and* μ *but independent of* h*.*

Proof. Clearly, the first estimate directly follows from the standard error estimate technique and Nitsche's duality trick (cf. [15, 63]). We now consider the second estimate. For any $w \in V_h$, it follows from (3.49) that

$$\begin{aligned} &\alpha_h(k, \pi_h v - \tilde{\Lambda}_h v, w) + (\mu\,(\pi_h v - \tilde{\Lambda}_h v), w)_h \\ &= \alpha_h(k, \pi_h v, w) + (\mu\,\pi_h v, w) - \alpha_h(k, \tilde{\Lambda}_h v, w) - (\mu\,\tilde{\Lambda}_h v, w)_h \\ &= \alpha_h(k, \pi_h v, w) + (\mu\,\pi_h v, w)_h - \alpha(k, v, w) - (\mu\, v, w) \\ &= \ [\alpha_h(k, \pi_h v, w) - \alpha(k, \pi_h v, w)] + [(\mu\,\pi_h v, w)_h - (\mu\,\pi_h v, w)] \\ &\quad - \alpha(k, v - \pi_h v, w) - (\mu\,(v - \pi_h v), w). \end{aligned}$$

Let k^I be the linear interpolation of k (similar notations will be used later). By (3.30), and the definitions of $\alpha_h(\cdot,\cdot,\cdot)$ and $\alpha(\cdot,\cdot,\cdot)$, we have that

$$\begin{aligned} &\alpha_h(k, \pi_h v, w) - \alpha(k, \pi_h v, w) \\ &= (k\nabla(\pi_h v), \nabla w)_h - (k\nabla(\pi_h v), \nabla w) \end{aligned}$$

$$
\begin{aligned}
&= \int_\Omega k^I \nabla(\pi_h v) \cdot \nabla w dx - \int_\Omega k \nabla(\pi_h v) \cdot \nabla w dx \\
&\le Ch \|\nabla(\pi_h v)\|_0 \|\nabla w\|_0 \\
&\le Ch \|v\|_2 \, |w|_1
\end{aligned}
$$

where C is dependent in the C^1-norm or H^1-norm of k. Similarly, defining μ^I, we have by (3.30) and Bramble-Hilbert Lemma (cf. [15, 63]),

$$
\begin{aligned}
&(\mu\,(\pi_h v, w)_h - (\mu \pi_h v, w) \\
&\quad = (\mu^I \, \pi_h v, w)_h - (\mu^I \, \pi_h v, w) + ((\mu^I - \mu)\, \pi_h v, w) \\
&\quad \le Ch^2 \sum_{e \in \mathcal{J}_h} \|\mu^I \pi_h v w\|_{H^2(e)} + Ch \|\pi_h v\|_0 \, \|w\|_0 \\
&\quad \le Ch^2 (\|\pi_h v\|_0 \|w\|_1 + \|\pi_h v\|_1 |w|_0 + |\pi_h v|_1 |w|_1) + Ch \|\pi_h v\|_0 \|w\|_0 \\
&\quad \le Ch^2 \|v\|_2 \, \|w\|_1 + Ch \|v\|_1 \, \|w\|_0
\end{aligned}
$$

where the constant C is dependent in the C^0-norm of μ. Moreover, from (3.30) and the definition of $\alpha(\cdot,\cdot,\cdot)$ (3.26),

$$
|\alpha(k, v - \pi_h v, w) + (\mu\,(v - \pi_h v),\ w)| \le Ch |v|_2 \|\nabla w\|_0 + Ch^2 |v|_2 \|w\|_0, \tag{3.50}
$$

where the constant C is dependent in the C^0-norm of k and μ. Therefore, we have obtained that

$$
\left| \alpha_h(k, \pi_h v - \tilde{\Lambda}_h v, w) + (\mu\,(\pi_h v - \tilde{\Lambda}_h v), w)_h \right|
$$

$$\le Ch\|v\|_2\,|w|_1 + Ch^2\|v\|_2\,\|w\|_1 + Ch|v|_1\,\|w\|_0.$$

In particular, taking $w = \pi_h v - \tilde{\Lambda}_h v$ in (3.51), we have that

$$\begin{aligned} |\pi_h v - \tilde{\Lambda}_h v|_1^2 &\le C(\alpha_h(k, \pi_h u - \tilde{\Lambda}_h v, w) + (\mu\,(\pi_h v - \tilde{\Lambda}_h v), w)_h) \\ &\le Ch^2\|v\|_2^2 + C(h^4+1)\|\pi_h v - \tilde{\Lambda}_h v\|_0^2 \end{aligned}$$

that is,

$$|\pi_h v - \tilde{\Lambda}_h v|_1 \le Ch\|v\|_2 + C(h^2+1)\|\pi_h v - \tilde{\Lambda}_h v\|_0. \qquad (3.51)$$

On the other hand, noting the auxiliary problem (3.46), we have that

$$\begin{aligned} (g, \pi_h v - \tilde{\Lambda}_h v) &= \alpha(\pi_h v - \tilde{\Lambda}_h v, \Phi) + (\mu\,(\pi_h v - \tilde{\Lambda}_h v), \Phi) \\ &= \alpha(\pi_h v - \tilde{\Lambda}_h v, \Phi - \Lambda_h\Phi) + (\mu\,(\pi_h v - \tilde{\Lambda}_h v), \Phi - \Lambda_h\Phi) \\ &\le C\|\nabla(\pi_h v - \tilde{\Lambda}_h v)\|_0\|\nabla(\Phi - \Lambda_h\Phi)\|_0 + C\|\pi_h v - \tilde{\Lambda}_h v\|_0\|\Phi - \Lambda_h\Phi\|_0 \\ &\le Ch|\pi_h v - \tilde{\Lambda}_h v|_1\|\Phi\|_2 + Ch^2\|\pi_h v - \tilde{\Lambda}_h v\|_0\|\Phi\|_2 \\ &\le Ch(|\pi_h u - \tilde{\Lambda}_h u|_1 + h\|\pi_h u - \tilde{\Lambda}_h\|_0)\|g\|_0. \end{aligned}$$

This together with (3.51) implies

$$\begin{aligned} \|\pi_h v - \tilde{\Lambda}_h v\|_0 &= \sup_{0 \ne g \in L^2(\Omega)} \frac{(g, \pi_h v - \tilde{\Lambda}_h)v}{\|g\|_0} \\ &\le Ch(|\pi_h v - \tilde{\Lambda}_h v|_1 + h\|\pi_h v - \tilde{\Lambda}_h v\|_0) \\ &\le Ch^2\|v\|_2 + Ch(h+1)\|\pi_h v - \tilde{\Lambda}_h v\|_0. \end{aligned}$$

Hence, which, together with (3.51), implies that, if h is sufficient small,

$$\|v - \tilde{\Lambda}_h v\|_0 + h\|(v - \tilde{\Lambda}_h v)\|_1 \leq Ch^2\|v\|_2,$$

Thus, we have proved Lemma 9.

Let u be the exact solution of the problem (3.24) and

$$\eta = u - \tilde{u} \equiv u - \tilde{\Lambda}_h u, \tag{3.52}$$

where $\tilde{\Lambda}_h$ is defined in (3.49). We then have

LEMMA 10 *Assume that all assumptions of Lemma* 9 *and* μ *has bounded first derivatives with respect to all of its variables over* $[0,T] \times [0,A_m) \times \Omega \times (0,+\infty)$. *Then there is a constant C, independent of h, such that, if* h *is sufficiently small,*

$$\|\eta\|_0 + h|\eta|_1 \leq Ch^2\|u\|_2 \tag{3.53}$$

$$\|\partial\eta\|_0 + h|\partial\eta|_1 \leq Ch^2(\|u\|_2 + \|\partial u\|_2) \tag{3.54}$$

where η *is defined by* (3.52) *and* ∂ *stands for* ∂_t *or* ∂_a *or* $\partial_\tau = \partial_t + \partial_a$.

Proof. Indeed, we only need show (3.54) since (3.53) can be obtained directly from Lemma 9. By differentiation of (3.24), we obtain that for any $w \in V_h$,

$$\alpha_h(k, \partial\tilde{u}, w) + (\mu\, \partial\tilde{u}, w)_h$$

$$= \alpha(k, \partial u, w) + (\mu\, \partial u, w) + \alpha(\partial k\, \nabla u, \nabla w)$$

$$+ (\partial k\, u, w) - \alpha_h(\partial k\, \nabla \tilde{u}, \nabla w)_h - (\partial \mu\, \tilde{u}, w)_h$$

that is,

$$\begin{aligned}
&\alpha_h(k, \partial(\pi_h u - \tilde{u}), w) + (\mu\, (\partial(\pi_h u - \tilde{u}), w)_h \\
&\quad = \; [\alpha_h(k, \partial(\pi_h u), w) + (\mu\, \partial(\pi_h u), w)_h - \alpha(k, \partial u, w) - (\mu\, \partial u, w)] \\
&\qquad [-(\partial \mu u, w) + (\partial \mu \tilde{u}, w)_h] + [-\, \alpha(\partial k\, \nabla u, \nabla w) + \alpha_h(\partial k\, \nabla \tilde{u}, \nabla w)_h]\,.
\end{aligned}$$

It is not hard to see that we have that by a similar argument used to show (3.51),

$$\begin{aligned}
&|\alpha_h(k, \partial(\pi_h u), w) + (\mu\, \partial(\pi_h u), w)_h - \alpha(k, \partial u, w) - (\mu\, \partial u, w)| \\
&\quad \leq \; Ch\|\partial u\|_2\|\nabla w\|_0 + Ch\|\partial u\|_2\|w\|_0
\end{aligned}$$

and by a similar arguments as that for (3.50),

$$\begin{aligned}
&[-(\partial \mu\; u, w) + (\partial \mu\; \tilde{u}, w)_h] \\
&\quad = \; (\partial \mu\; (\tilde{u} - u), w) - (\partial \mu\; \tilde{u}, w) + ([\partial \mu]^I\; \tilde{u}, w)_h \\
&\quad \leq \; Ch^2\|u\|_2\|w\|_0 + (([\partial \mu]^I - \partial \mu)\tilde{u}, w) \\
&\qquad +([\partial \mu]^I \tilde{u}, w)_h - ([\partial \mu]^I \tilde{u}, w) \\
&\quad \leq \; Ch(h+1)\|u\|_2\|w\|_0 + Ch^2\|u\|_2(|w|_1 + \|w\|_0)
\end{aligned}$$

$$\leq\ Ch^2\|u\|_2|w|_1 + Ch\|u\|_2\|w\|_0.$$

Also, from Lemma 9 and (3.30),

$$\begin{aligned}
&[-\alpha(\partial k,\ \nabla u, \nabla w) + \alpha_h(\partial k,\ \nabla \tilde{u}, \nabla w)] \\
&\quad = -(\partial k \nabla u, \nabla w) + ([\partial k]^I \nabla(\tilde{u} \nabla w)_h \\
&\quad = (\partial k \nabla(\tilde{u} - u), \nabla w) + (([\partial k]^I - \partial k)\ \nabla \tilde{u}, \nabla w) \\
&\quad \leq C|\tilde{u} - u|_1|w|_1 + Ch|\tilde{u}|_1|w|_1 \\
&\quad \leq Ch\|u\|_2|w|_1.
\end{aligned}$$

Therefore, we have obtained that

$$\begin{aligned}
&|\ \alpha_h(k, \partial(\pi_h u - \tilde{u}), w) + (\mu\ (\partial(\pi_h u - \tilde{u}), w)_h\ | \\
&\quad \leq\ Ch\|u\|_2|w|_1 + Ch\|u\|_2\|w\|_0\,,
\end{aligned}$$

in particular, taking $w = \partial_\tau(\pi_h u - \tilde{u})$, which implies,

$$|\partial(\pi_h u - \tilde{u})|_1 \leq Ch\|u\|_2 + C\|\partial(\pi_h u - \tilde{u})\|_0\,. \tag{3.55}$$

Moreover, by the standard duality argument (cf. [15, 63]), (indeed, by a completely similar argument used in the proof of Lemma 9),

$$\begin{aligned}
\|\partial(\pi_h u - \tilde{u})\|_0 &\leq Ch|\partial(\pi_h u - \tilde{u})|_1 + Ch^2\|\partial(\pi_h u - \tilde{u})\|_0 \\
&\leq Ch^2\|u\|_2 + Ch\|\partial(\pi_h u - \tilde{u})\|_0 .
\end{aligned}$$

Hence, which together with (3.55) implies that, if h is sufficient small,

$$\|\partial(\pi_h u - \tilde{u})\|_0 + h|\partial(\pi_h u - \tilde{u})|_1 \leq Ch^2(\|u\|_2 + \|\partial u\|_2). \tag{3.56}$$

Notice that $\partial\eta = \partial(u - \pi_h u) + \partial(\pi_h u - \tilde{u})$, then, by the interpolation approximate property, (3.56) and the triangle inequality, we can get (3.54). This completes the proof.

We now ready to consider the convergence error estimate for numerical approximate problem (3.27). Let (u, P) satisfy the problem (3.24) and $(u_h^{n,j}, P_h^n)$ satisfy the numerical approximate problem (3.27). We denote by

$$\begin{aligned}
&u^{n,j}(x) = u(t_n, a_j, x) \\
&P_h^n(x) = P(t_n, x) \\
&\tilde{u}^{n,j}(x) = \tilde{\Lambda}_h u^{n,j} \\
&\eta^{n,j} = u^{n,j} - \tilde{u}^{n,j} \\
&\xi^{n,j} = \tilde{u}^{n,j} - u_h^{n,j}
\end{aligned} \tag{3.57}$$

moreover, for

$$\xi^n = (\xi^{n,0}, \xi^{n,1}, \cdots, \xi^{n,N_a}), \qquad \xi = (\xi^0, \xi^1, \cdots, \xi^{N_a}),$$

we introduce the following norms:

$$\begin{aligned} \|\xi^n\|_{\ell^p(h)} &= (\sum_j \|\xi^{n,j}\|_h^p \tau)^{1/p} \\ \|\xi^n\|_{\ell^p(H^r)} &= (\sum_j \|\xi^{n,j}\|_{H^r}^p \tau)^{1/p} \\ \|\xi\|_{\ell^{p,q}(H^r)} &= (\sum_j \|\xi^n\|_{\ell^p(H^r)}^q \tau)^{1/q} \end{aligned} \tag{3.58}$$

where, if $q = \infty$, the *sum* is replaced by the *maximum*. Then, we can have the error estimate concerning the numerical problem(3.27).

THEOREM 7 *Assume that all the assumptions of Lemma* 10 *hold and* $u \in L^2([0,T] \times [0, A_m], V \cap W^{2,\infty}(\Omega))$. *Also, let* $u^{n,j} \in V \cap W^{2,\infty}(\Omega)$, $u_t^{n,j}$, $u_a^{n,j} \in H^2(\Omega)$, $u_{tt}^{n,j}$, $u_{aa}^{n,j}$, $u_{ta}^{n,j} \in L^2(\Omega)$. *Then, for sufficiently small* τ *and* h, *we have the following error estimates:*

$$\|u - u_h\|_{\ell^{\infty,2}(L^2)} \leq C(\tau + h^2)$$

$$\|\nabla(u - u_h)\|_{\ell^{2,2}(L^2)} \leq C(\tau + h)$$

$$\|P - P_h\|_{\ell^2(L^2)} \leq C(\tau + h^2)$$

where we understand that, as in (3.57),

$$u = (u^0, u^1, \cdots, u^{N_t})$$

$$u^n = (u^{n,0}, u^{n,1}, \cdots, u^{n,N_a})$$

$$P = (P^0, P^1, \cdots, P^{N_t})$$

and C *is a generic constant, independent of* τ *and* h.

Proof. Notice that

$$u^{n,j} - u_h^{n,j} = \eta^{n,j} + \xi^{n,j}, \tag{3.59}$$

and it follows from Lemma 10 that

$$\|\eta^{n,j}\|_0 + h|\eta^{n,j}|_1 \le Ch^2 \|u^{n,j}\|_2 \le Ch^2 \tag{3.60}$$

$$\|\partial\eta^{n,j}\|_0 + h|\partial\eta^{n,j}|_1 \le Ch^2(\|u^{n,j}\|_2 + \|\partial u^{n,j}\|_2) \le Ch^2 \tag{3.61}$$

where ∂ is defined in Lemma 10. So, it only remains to estimate $\xi^{n,j}$. It follows from (3.24) (3.49) and (3.57) that, for any $w \in V_h$,

$$\begin{aligned}
&(\tilde{\partial}_\tau \xi^{n,j},\, w)_h + \alpha_h(\tilde{k}_h^{n-1}, \xi^{n,j}, w) + (\tilde{\mu}_h^{n-1,j}\, \xi^{n,j},\, w)_h \\
&\quad = (\tilde{\partial}_\tau \tilde{u}^{n,j},\, w)_h + \alpha_h(\tilde{k}_h^{n-1}, \tilde{u}^{n,j},\, w)_h + (\tilde{\mu}_h^{n-1,j}\, \tilde{u}^{n,j},\, w)_h \\
&\quad = (\tilde{\partial}_\tau \tilde{u}^{n,j},\, w)_h + \alpha_h(k^n, \tilde{u}^{n,j},\, w)_h + (\mu^{n,j}\, \tilde{u}^{n,j},\, w)_h
\end{aligned}$$

$$
\begin{aligned}
&\quad + \alpha_h((\tilde{k}_h^{n-1} - k^n), \tilde{u}^{n,j},\, w) + ((\tilde{\mu}_h^{n-1,j} - \mu^{n,j})\, \tilde{u}^{n,j},\, w)_h \\
&= (\tilde{\partial}_\tau \tilde{u}^{n,j},\, w)_h + \alpha(k^n, \tilde{u}^{n,j},\, w) + (\mu^{n,j}\, \tilde{u}^{n,j},\, w) \\
&\quad + \alpha_h((\tilde{k}_h^{n-1} - k^n), \tilde{u}^{n,j},\, w) + ((\tilde{\mu}_h^{n-1,j} - \mu^{n,j})\, \tilde{u}^{n,j},\, w)_h \\
&= [\, (\tilde{\partial}_\tau \tilde{u}^{n,j},\, w)_h - (\partial_\tau u^{n,j},\, w)\,] + \alpha_h((\tilde{k}_h^{n-1} - k^n),\, \tilde{u}^{n,j},\, w) \\
&\quad + ((\tilde{\mu}_h^{n-1,j} - \mu^{n,j})\, \tilde{u}^{n,j},\, w)_h\,.
\end{aligned}
$$

We now estimate three terms in the above right hand side. First, noting that

$$
\begin{aligned}
(\tilde{\partial}_\tau \tilde{u}^{n,j},\, w)_h - (\partial_\tau u^{n,j},\, w) \;&=\; [\, (\tilde{\partial}_\tau \tilde{u}^{n,j},\, w)_h - (\tilde{\partial}_\tau \tilde{u}^{n,j},\, w)\,] \\
&+ (\tilde{\partial}_\tau(\tilde{u}^{n,j} - u^{n,j}),\, w) + (\tilde{\partial}_\tau u^{n,j} - \partial_\tau u^{n,j},\, w),
\end{aligned}
$$

we have that, from (3.24) (3.25) (3.26) (3.49) (3.57), Bramble-Hilbert Lemma (cf. [15, 63]) and by a direct computation,

$$
\begin{aligned}
&|\, (\tilde{\partial}_\tau \tilde{u}^{n,j},\, w)_h - \; (\tilde{\partial}_\tau \tilde{u}^{n,j},\, w)\,| \\
&\le\; Ch^2 |\tilde{\partial}_\tau \tilde{u}^{n,j}\, w|_2 \\
&\le\; Ch^2 \|\nabla\, (\tilde{\partial}_\tau \tilde{u}^{n,j})\|_0\, \|\nabla\, w\|_0 \\
&\le\; Ch^2 (\|\nabla(\tilde{\partial}_\tau(\tilde{u}^{n,j} - u^{n,j}))\|_0 + + \|\nabla(\tilde{\partial}_\tau u^{n,j})\|_0)\; \|\nabla\, w\|_0 \\
&\le\; Ch^2 (h+1)(\|\tilde{u}_t^{n,j}\|_2 + \|\tilde{u} i_t^{n-1,j-1}\|_2 + \|u_t^{n,j}\|_1) \|\nabla\, w\|_0 \\
&\le\; Ch^2 (h+1) \|\nabla\, w\|_0\,,
\end{aligned}
$$

$$\begin{aligned} |\,(\tilde{\partial}_\tau(\tilde{u}^{n,j} - u^{n,j}),\, w)\,| &\leq \|\bar{\partial}_\tau(\tilde{u}^{n,j} - u^{n,j})\|_0 \|w\|_0 \\ &\leq Ch^2(\|u_t^{n,j}\|_2 + \|u_t^{n-1,j-1}\|_2)\|w\|_0 \\ &\leq Ch^2\|w\|_0 \end{aligned}$$

and

$$\begin{aligned} |(\tilde{\partial}_\tau u^{n,j} - \partial_\tau u^{n,j},\, w)| &\leq \|\tilde{\partial}_\tau u^{n,j} - \partial_\tau u^{n,j}\|_0 \|w\|_0 \\ &\leq C\tau(\|u_{tt}\|_0 + \|u_{ta}\|_0 + \|u_{aa}\|_0)\|w\|_0 \\ &\leq C\tau\|w\|_0. \end{aligned}$$

Hence,

$$\begin{aligned} &|\,(\tilde{\partial}_\tau \tilde{u}^{n,j},\, w)_h - (\tilde{\partial}_\tau \tilde{u}^{n,j},\, w)\,| \\ &\leq Ch^2(h+1)\|\nabla\, w\|_0 + C(h^2+\tau)\|w\|_0. \end{aligned} \tag{3.62}$$

Second, we have that, from the linear interpolation error estimate (cf. [15, 63]),

$$\begin{aligned} |\alpha_h(\tilde{k}_h^{n-1} - k^n, \tilde{u}^{n,j}, w)| &= |([\tilde{k}_h^{n-1} - k^n]^I\, \nabla \tilde{u}^{n,j},\, \nabla w)_h| \\ &\leq C(h + \|\tilde{k}_h^{n-1} - k^n\|_0)\|\nabla \tilde{u}^{n,j}\|_{0,\infty}\|\nabla w\|_0 \\ &\leq C(h^2 + \|\tilde{k}_h^{n-1} - k^n\|_0)\|\nabla w\|_0\,. \end{aligned} \tag{3.63}$$

Third, by an elementary computation,

$$
\begin{aligned}
&((\tilde{\mu}_h^{n-1,j} - \mu^{n,j})\tilde{u}^{n,j},\ w)_h \\
&= (\,[\tilde{\mu}_h^{n-1,j} - \mu^{n,j}]^I\ \tilde{u}^{n,j},\ w)_h \\
&\leq \Big[(\,[\tilde{\mu}_h^{n-1,j} - \mu^{n,j}]^I\ \tilde{u}^{n,j},\ w)_h - ([\tilde{\mu}_h^{n-1,j} - \mu^{n,j}]^I\ \tilde{u}^{n,j},\ w)\Big] \\
&\quad + (\,[\tilde{\mu}_h^{n-1,j} - \mu^{n,j}]^I\ \tilde{u}^{n,j},\ w).
\end{aligned}
$$

Therefore, from Bramble-Hilbert Lemma and the linear interpolation error estimate (cf. [15, 63]), we have that

$$
\begin{aligned}
&\Big|\,(\,[\tilde{\mu}_h^{n-1,j} - \ \mu^{n,j}]^I\ \tilde{u}^{n,j}\ w)_h - (\,[\tilde{\mu}_h^{n-1,j} - \mu^{n,j}]^I\ \tilde{u}^{n,j}\ w)\,\Big| \\
&\leq Ch^2|(\,[\tilde{\mu}_h^{n-1,j} - \mu^{n,j}]^I\ \tilde{u}^{n,j}\ w)|_2 \\
&\leq Ch^2\|\tilde{u}^{n,j}\|_1\,(\|w\|_0 + \|\nabla w\|_0)\,,
\end{aligned}
$$

$$
\begin{aligned}
|(\,[\tilde{\mu}_h^{n-1,j} - \mu^{n,j}]^I\ \tilde{u}^{n,j},\ w)| &\leq \|\tilde{u}^{n,j}\|_{0,\infty}\|\,[\tilde{\mu}_h^{n-1,j} - \mu^{n,j}]^I\|_0\|w\|_0 \\
&\leq C(h^2 + \|\tilde{\mu}_h^{n-1,j} - \mu^{n,j}\|_0)\|w\|_0.
\end{aligned}
$$

Hence,

$$
\begin{aligned}
&|((\tilde{\mu}_h^{n-1,j} - \mu^{n,j})\tilde{u}^{n,j},\ w)_h| \\
&\leq Ch^2(\|w\|_0 + \|\nabla w\|_0) + C\|\tilde{\mu}_h^{n-1,j} - \mu^{n,j}\|_0\|w\|_0. \qquad (3.64)
\end{aligned}
$$

On the other hand, notice that

$$\begin{aligned}\|P^n - P^{n-1}\|_0 &= \|\int_0^{A_m} (u(t_n, a, x) - u(t_{n-1}, a, x))\, da\|_0 \\ &\leq C(A_m, u_t)\tau = O(\tau) \qquad (3.65)\end{aligned}$$

and

$$\begin{aligned}P^n - P^n_h &= \frac{1}{2}(u^{n,0} - u_h^{n,0})\tau + \sum_{j=1}^{N_a-1}(u^{n,j} - u_h^{n,j})\tau + O(\tau) \\ &= \frac{1}{2}(\xi^{n,0} + \eta^{n,0})\tau + \sum_{j=1}^{N_a-1}(\xi^{n,j} + \eta^{n,j})\tau + O(\tau) \\ &\leq \sum_{j=0}^{N_a-1}(\xi^{n,j} + \eta^{n,j})\tau + O(\tau)\end{aligned}$$

which, together with (3.60) (3.61), implies,

$$\|P^n - P^n_h\|_0 \leq \|\xi^n\|_{\ell^1(L^2)} + O(h^2 + \tau). \qquad (3.66)$$

Then, by a direct computation using the mean value theorem, we can obtain

$$\begin{aligned}\|\tilde{k}_h^{n-1} - k^n\|_0 &= \|k(t_n, x, P_h^{n-1}) - k(t_n, x, P^n)\|_0 \\ &\leq C\|P_h^{n-1} - P^n\|_0 \\ &\leq C\|\xi^{n-1}\|_{\ell(L^2)} + O(h^2 + \tau)\end{aligned}$$

and

$$\begin{aligned}\|\tilde{\mu}_h^{n-1,j} - \mu^{n,j}\|_0 &= \|\mu(t_n, a_j, x, P_h^{n-1}) - \mu((t_n, a_j, x, P^n)\|_0 \\ &\leq C\|P_h^{n-1} - P^n\|_0 \\ &\leq C\|\xi^{n-1}\|_{\ell(L^2)} + C(h^2 + \tau)\,.\end{aligned}$$

Then, (3.63) and (3.64) can be rewritten as:

$$\begin{aligned}|\alpha_h(\tilde{k}_h^{n-1} - k^n, \tilde{u}^{n,j}, w)| &\leq C(\|\xi^{n-1}\|_{\ell(L^2)} + h^2 + \tau)\|\nabla w\|_0 \\ |((\tilde{\mu}_h^{n-1,j} - \mu^{n,j})\tilde{u}^{n,j}\, w)_h| &\leq C(\|\xi^{n-1}\|_{\ell(L^2)} + h^2 + \tau)\|w\|_0.\end{aligned}$$

Therefore, combining the above two estimates and (3.62), we have that

$$\begin{aligned}&\left|\, (\tilde{\partial}_\tau \xi^{n,j},\, w)_h + \alpha_h(\xi^{n,j},\, w) + (\tilde{\mu}^{n-1,j}\, \xi^{n,j},\, w)_h\right| \\ &\leq C(\|\xi^{n-1}\|_{\ell^1(L^2)} + h^2 + \tau)(\|w\|_0 + \|\nabla w\|_0) \\ &\leq C(\|\xi^{n-1}\|_{\ell^1(L^2)} + h + \tau)(\|w\|_h + \|\nabla w\|_0)\,. \qquad (3.67)\end{aligned}$$

In particular, taking $w = \xi^{n,j}$ and observing that

$$(\tilde{\partial}_\tau \xi^{n,j},\, \xi^{n,j}) \geq \frac{1}{2\tau}(\|\xi^{n,j}\|_h^2 - \|\xi^{n-1}\|_h^2),$$

we then have that

$$\begin{aligned}
&\frac{1}{2\tau}(\|\xi^{n,j}\|_h^2 - \|\xi^{n-1}\|_h^2) + \ k_0\|\nabla\xi^{n,j}\|_0^2 \\
&\leq\ C(\|\xi^{n-1}\|_{\ell^1(L^2)} + h^2 + \tau)(\|\xi^{n,j}\|_h + \|\nabla\xi^{n,j}\|_0) \\
&\leq\ \frac{k_0}{4}\|\nabla\xi^{n,j}\|_0^2 + \frac{1}{4}\|\xi^{n,j}\|_h^2 + C(h^4 + \tau^2); \qquad (3.68)
\end{aligned}$$

that is,

$$\begin{aligned}
&\|\xi^{n,j}\|_h^2 - \|\xi^{n-1}\|_h^2 + \ \frac{3k_0}{2}\|\nabla\xi^{n,j}\|_0^2\tau \\
&\leq\ C\tau\|\xi^{n,j}\|_h^2 + C\tau\|\xi^{n-1}\|_{\ell^1(L^2)}^2 + C(h^4 + \tau^2)\tau.
\end{aligned} \qquad (3.69)$$

Summing it over $1 \leq j \leq N_a$ and using Schwarz's inequality, we obtain

$$\begin{aligned}
&\frac{1}{\tau}(\|\xi^n\|_{\ell^2(h)}^2 - \|\xi^{n-1}\|_{\ell^2(h)}^2 - \|\xi^{n,0}\|_h^2) + \frac{3k_0}{2}\|\nabla\xi^{n,j}\|_{\ell^2(L^2)}^2 \\
&\leq\ C\|\xi^n\|_{\ell^2(h)}^2 + C\|\xi^{n-1}\|_{\ell^2(h)}^2 + C(h^4 + \tau^2).
\end{aligned}$$

Hence,

$$\begin{aligned}
&\|\xi^n\|_{\ell^2(h)}^2 - \|\xi^{n-1}\|_{\ell^2(h)}^2 + \frac{3k_0}{2}\tau\|\nabla\xi^{n,j}\|_{\ell^2(L^2)}^2 \\
&\leq\ \tau\|\xi^{n,0}\|_h^2 + C\tau(\|\xi^n\|_{\ell^2(h)}^2 + \|\xi^{n-1}\|_{\ell^2(h)}^2) + C(h^4 + \tau^2)\tau.
\end{aligned} \qquad (3.70)$$

It now remains to estimate $\|\xi^{n,0}\|_h$. By (3.24) and (3.27), we have

$$u^{n,0} - h_h^{n,0} \ = \ \frac{1}{2}\beta^{n,0}u^{n,0}\tau + \sum_{j=1}^{N_a-1}\beta^{n,j}u^{n,j}\tau + O(\tau)$$

$$
\begin{aligned}
& -\frac{1}{2}\tilde{\beta}_h^{n-1,0}u_h^{n,0}\tau+\sum_{j=1}^{N_a-1}\tilde{\beta}_h^{n-1,j}u_h^{n,j}\tau \\
= \; & \frac{1}{2}\beta^{n,0}(u^{n,0}-u_h^{n,0})\tau+\sum_{j=1}^{N_a-1}\beta^{n,j}(u^{n,j}-u_h^{n,j})\tau \\
& +\frac{1}{2}(\beta^{n,0}-\tilde{\beta}_h^{n-1,0})\tau+\sum_{j=1}^{N_a-1}(\beta^{n,j}-\tilde{\beta}_h^{n-1,j})u_h^{n,j}\tau+O(\tau)
\end{aligned}
$$

which implies

$$
|u^{n,0}-h_h^{n,0}|\leq\sum_{j=0}^{N_a-1}|\beta^{n,j}(u^{n,j}-u_h^{n,j})|\tau+\sum_{j=0}^{N_a-1}|(\beta^{n,j}-\tilde{\beta}_h^{n-1,j})u_h^{n,j}|\tau+O(\tau).
$$

By some direct computations, we have

$$
|\,\beta^{n,j}(u^{n,j}-u_h^{n,j})\,| \;\leq\; \bar{\beta}|u^{n,j}-u_h^{n,j}\,| \;\leq\; \bar{\beta}(|\xi^{n,j}|+|\eta^{n,j}|),
$$

$$
\begin{aligned}
|\,(\beta^{n,j}-\tilde{\beta}_h^{n-1,j})u_h^{n,j}\,| \;&\leq\; C|\beta(t_n,a_j,x,P^n)-\beta(t_n,a_j,x,P_h^{n-1})| \\
&\leq\; C|\,P^n-P_h^{n-1}\,|\,.
\end{aligned}
$$

Combining the above three inequalities and (3.65) (3.66), we have

$$
\begin{aligned}
& \|u^{n,0}-h_h^{n,0}\|_0 \\
& \leq\; C(\|\xi^n\|_{\ell^1(L^2)}+\|\eta^{n,j}\|_{\ell^1(L^2)}+\|P^n-P_h^{n-1}\|_0)+C(h^2+\tau) \\
& \leq\; C(\|\xi^n\|_{\ell^1(L^2)}+\|\xi^{n-1}\|_{\ell^1(L^2)})+C(h^2+\tau)\,. \qquad (3.71)
\end{aligned}
$$

Hence, we have from (3.57) (3.58) that

$$\begin{aligned}\frac{1}{2}\|\xi^{n,0}\|_h &\le \|\xi^{n,0}\|_0 = \|u^{n,j} - u_h^{n,j} + \xi^{n-1,j}\|_0 \\ &\le C(\|\xi^n\|_{\ell^1(L^2)} + \|\xi^{n-1}\|_{\ell^1(L^2)}) + C(h^2+\tau) \\ &\le C(\|\xi^n\|_{\ell^1(h)} + \|\xi^{n-1}\|_{\ell^1(h)}) + C(h^2+\tau)\,. \end{aligned} \tag{3.72}$$

Plugging this into (3.70), we have

$$\begin{aligned}&(1-C\tau)\|\xi^n\|^2_{\ell^2(h)} + \frac{3k_0}{2}\tau\|\nabla\xi^n\|^2_{\ell^2(L^2)} \\ &\le (1+C\tau))\|\xi^{n-1}\|^2_{\ell^2(h)} + C(h^4+\tau^2)\tau. \end{aligned} \tag{3.73}$$

Therefore, summing over $1 \le n \le K < N_t$ and using the Gronwall inequality (cf. [34, 90]), we have that, if τ and h is sufficiently small,

$$\|\xi^K\|^2_{\ell^2(h)} + \frac{3k_0}{2}\|\nabla\xi|^2_{\ell^2(L^2)} \le C\|\xi^0\|^2_{\ell^2(h)} + C\|\xi^0\|^2_{\ell^2(h)} + C(h^4+\tau^2)$$

which implies that

$$\|\xi^K\|^2_{\ell^2(L^2)} + k_0\|\nabla\xi|^2_{\ell^2(L^2)} \le C\|\xi^0\|^2_{\ell^2(L^2)} + C\|\xi^0\|^2_{\ell^2(L^2)} + C(h^4+\tau^2). \tag{3.74}$$

Noting that the choice of $u_h^{0,j}$ in the approximate problem (3.27), we have

$$\|\xi^0\|_{\ell^2(L^2)} = \|u_0 - u_h^{0,j} - \eta^{0,j}\|_{\ell^2(L^2)}$$

$$
\begin{aligned}
&\le \|u_0 - u_h^{0,j}\|_{\ell^2(L^2)} + \|\eta^{0,j}\|_{\ell^2(L^2)} \\
&\le Ch^2 \qquad (3.75)
\end{aligned}
$$

which, together with (3.74), implies that

$$\|\xi\|_{\ell^{\infty,2}(L^2)} + \|\nabla\xi\|_{\ell^{2,2}(L^2)} \le C(\tau + h^2). \qquad (3.76)$$

Hence, the third estimate of Theorem 7 can be obtained immediately from (3.66) and (3.76). Also, from (3.59) (3.60) (3.61) and (3.76), and by triangle inequality, we can obtain the first two estimates of Theorem 7. Thus, we have completed the proof.

Furthermore, it follows from Theorem 7 and its proof that we can have immediately the following Corollary.

COROLLARY 1 *Under the same assumptions as Theorem 7, we have that*

$$
\begin{aligned}
\|u^{n,j} - u_h^{n,j}\|_0 &\le C(\tau + h^2), \\
\|\nabla(u^{n,j} - u_h^{n,j})\|_0 &\le C(\tau + h), \\
\|P^n - P_h^n\|_0 &\le (\tau + h^2).
\end{aligned}
$$

Theorem 7 and Corollary 1 shows the error estimates of the numerical approximate solutions are optimal in the numerical analysis view point.

Remark 3.2.2.1: From the above proofs and the definition of local truncation error (cf. [76, 88]), it is not difficult to see by a standard analysis as in [76, 88] that the local truncation error of the numerical scheme (3.27) has the accuracy of $O(\tau^2 + h^2)$, that is,

$$\|u^{n,j} - u_h^{n,j}\|_0 + \|P^n - P_h^n\|_0 = O(\tau^2 + h^2).$$

Remark 3.2.2.2: Consider a new problem which is modified from the problem (3.23) by using the following simple initial condition (3.77) to replace the fourth equality of (3.23) or the third equality of (3.24).

$$u(t, 0, x) = B(t, x) \quad (given). \tag{3.77}$$

Then, we can construct a numerical approximate problem of this new problem which is modified from the numerical approximation problem (3.27) by using the following equation (3.79) to replace the fourth equation of (3.27).

$$u_h^{n,0} = \pi_h u^{n,0} = \pi_h(B(t_n, x)). \tag{3.78}$$

It is not hard to see that (3.69) is still true for the above new problem and its numerical approximate problem. However, the estimate of $\|\xi^{n,0}\|_h$ is obtained as follows.

$$\begin{aligned}\frac{1}{2}\|\xi^{n,0}\|_h &\le \|\xi^{n,0}\|_0 = \|u^{n,0} - u_h^{n,0} + \eta^{n,0}\|_0 \\ &\le \|B(t_n,x) - \pi_h(B(t_n,x))\|_0 + \|\eta^{n,0}\|_0 \\ &\le C(h^2+\tau).\end{aligned}$$

Plugging this into (3.69), we can get the same results of Theorem 7 and Corollary 1. This means Theorem 7 and Corollary 1 are still true for the new problem and its numerical approximate problem as above.

Remark 3.2.2.3: Theorem 7 and Corollary 1 can be extended to the case of the flux $\mathcal{D}$ explicitly including an advection term as in (1.11), that is,

$$\mathcal{D} = k\,\nabla u - \mathbf{q}\,u. \tag{3.79}$$

Then, the related bilinear form in the numerical approximate problem is as

$$a_h(k,u,v) - (\mathbf{q}\,u,\ \nabla v)_h + (\mu\,u,\ v)_h + \frac{1}{\tau}(u,\ v)_h. \tag{3.80}$$

Clearly, the corresponding liner system in (3.32) is not symmetric. The bilinear form (3.80) still could be coercive if $\mathbf{q}$ is not large or μ is large enough. Otherwise, we have to choose τ small enough to make the bilinear form (3.80) to be coercive. Therefore, from the proof of Theorem 7, Theorem 7 and Corollary 1 are still true for the model with both diffusion and advection theoretically if the bilinear form (3.80) is coercive, especially, if τ is very small. On the other hand, theoretically, we may assume that (3.80) is always coercive since we can use the transferring techniques of **Remark 2.3.1** and **Remark 2.3.2** to transfer the original problem into a similar one but by using $\mu + C$ to replace μ, where C, a constant, which could be chosen large enough. However, for a general auxiliary age structured population problem (II) (3.23) plus with advection term, which may be large, it is not easy to construct a practical numerical numerical scheme by using the above techniques. Thus, in real computations, the above technique cannot be applied usually. The computational work would be increased dramatically if a small τ is taken. Also, it is difficult to choose a C of the transformation since $\mathbf{q}$ and μ are usually dependent on u. A common technique to overcome this difficulty is to apply an *upwind* scheme to discretize the advection term (see **Remark 3.2.2.4**).

Remark 3.2.2.4: As we have mentioned in **Remark 3.2.2.3**, for many problems with both diffusion and advection in the real world, μ is usually small and $\mathbf{q}$ may be very large. Therefore, in order to apply the methods and results of this section into these real problems, we have to either choose a small time-age step τ or use the transferring techniques of **Remark 2.3.1** and **Remark 2.3.2**. However, it is well-known that a small τ will increase a lot the computation work and the constant C of the transformation is difficult to determine. This at least means that we cannot apply the above scheme to such real problems directly. In fact, we usually need to use a technique of *upwind scheme* for the advection term to modify the scheme defined in this subsection. In precisely, we choose a *upwind scheme*, $R_h(\mathbf{q}\,u,\ \nabla v)$, to replace $(\mathbf{q}\,u,\ \nabla v)_h$ of (3.80), that is, the approximate bilinear form (3.80) is modified into the following *upwind scheme*

$$\alpha_h(k,u,v) - R_h(\mathbf{q}\,u,\ \nabla v) + (\mu\,u,\ v)_h + \frac{1}{\tau}(u,\ v)_h. \tag{3.81}$$

The detailed definition of *upwind scheme* $R_h(\mathbf{q}\,u,\ \nabla v)$, which has several different formats, can be found in the book [56, 60]. For the 1-*dimension* case, a *upwind scheme* will be given in Chapter 4 and Chapter 5. The *upwind scheme* guarantees that not only the bilinear form (3.81) is coercive but also its matrix is an *M-Matrix* even if we don't choose a small τ for the problems with a large $\mathbf{q}$. However, it is not trivial to extend Theorem 7 and Corollary 1 into the above *upwind scheme*; we need some special techniques. The numerical analysis for the *upwind scheme* will be discussed later.

3.2.3 Numerical Scheme for Age structured Population Problem (III)

This subsection considers the auxiliary age structured population problem (III) defined in the Section 2.3 of Chapter 2. The problem is a mixed type of nonlinear partial differential problem. In fact, it is a kind of combination of the auxiliary age structured population problem (I), i.e., (3.10) and the auxiliary age structured population problem (II), i.e., (3.23), which describes that the model organisms do not move in the embryonic stage, i.e., age interval $[0, J]$, but have diffusive and advective movement in the older life stage, i.e. age interval $(J, A_m]$. The basic technique to construct its numerical approximate scheme is to apply the numerical approximate schemes of the auxiliary age structured population problem (I), i.e., (3.10) and auxiliary age structured population problem (II), i.e., (3.23), to the corresponding parts of the unstructured population problem (III), which have applied the characteristic finite difference discretization for time-age domain and the linear finite element approximation for the spatial domain. Thus, based on the numerical schemes and analyses for the problem (3.10) and (3.23), we have constructed a numerical approximate scheme for the auxiliary age structured population problem (III) and we also have given a numerical analysis for the numerical scheme. The analyses have shown that the numerical approximate scheme has a unique biological approximate solution, that means that the approximate solution is always nonnegative, and an optimal convergence error estimate is obtained from the numerical analysis view point.

For convenience, we restate the auxiliary age structured problem (III) as follows

$$\begin{gathered}\frac{\partial u}{\partial t}+\frac{\partial u}{\partial a}+= \ -\mu\, u \\ \text{for } \ t\in(0,T], \ a\in(0,J], \ x\in\Omega\end{gathered} \tag{3.82}$$

$$\begin{gathered}\frac{\partial u}{\partial t}+\frac{\partial u}{\partial a}-\nabla\cdot(k\nabla\, u)= \ -\mu\, u \\ \text{for } \ t\in(0,T], \ a\in(J,A_m], \ x\in\Omega\end{gathered} \tag{3.83}$$

$$
\begin{aligned}
& k\frac{\partial u}{\partial \nu} = 0 \quad \text{or} \quad u = 0, \;\; x \in \partial\Omega \\
& u(0,a,x) = \; u_0(a,x) \\
& u(t,0,x) = \; \int_0^{A_m} \beta\, u(t,a,x)\, da,
\end{aligned}
\tag{3.84}
$$

where μ , k , β and P are defined the last subsection. Moreover, if extending k to $\tilde{k}$ as previous,we rewrite (3.82) and (3.83) as a unified form.

$$
\begin{aligned}
& \frac{\partial u}{\partial t} + \frac{\partial u}{\partial a} - \nabla \cdot (\tilde{k}\, \nabla u) = \; -\mu\, u \\
& \qquad\qquad \text{for} \quad t \in (0,T], \; a \in [0, A_m], \; x \in \Omega \\
& \tilde{k}\, \frac{\partial u}{\partial \nu} = 0 \quad \text{or} \quad u = 0, \quad \text{on} \;\; \partial\Omega \\
& u(0,a,x) = \; u_0(a,x) \\
& u(t,0,x) = \; \int_0^{A_m} \beta\, u(t,a,x)\, da.
\end{aligned}
\tag{3.85}
$$

Therefore, the problem (3.85) is a nonlocal initial-boundary nonlinear partial differential equation with discontinuous coefficient $\tilde{k}$. We also need to recall its the weak formulation: find $u \in L^2(\, (0,T] \times [0, A_m],\, V\,)$, such that

$$
(\partial_\tau u,\; w) + \alpha(\tilde{k}, u, w) = -(\mu\, u,\; w), \qquad \forall\, w \in V. \tag{3.86}
$$

We now construct a numerical discretization approximate scheme for (3.86). We use the same the finite difference partition and finite element partition $\mathcal{J}_h$ for

$(0,T] \times [0,A_m]$ and Ω, and same finite element space V_h as previous; moreover assume that there is an integer N_j such that $J = N_j \cdot \tau$ and $\mathcal{J}_h$ is weak acute. Then we can define a numerical approximate scheme for the problem (3.85), i.e., (3.86), as follows. For $1 \le j \le N_a$ and $1 \le n \le N_t$, seeking

$$u_h^{n,j} = \sum_{b \in \mathcal{N}_h} u_h^{n,j}(b) \varphi_b \in V_h \tag{3.87}$$

such that

$$\begin{aligned} \frac{u_h^{n,j}(b) - u_h^{n-1,j-1}(b)}{\tau} &= -\tilde{\mu}_h^{n-1,j}(b)\, u_h^{n,j}(b), \\ &\forall\, b \in \mathcal{N}_h,\ 1 \le j \le N_j,\ 1 \le n \le N_t \end{aligned} \tag{3.88}$$

$$\begin{aligned} (\tilde{\partial}_\tau u_h^{n,j}, w)_h \ + \alpha_h(\tilde{k}_h^{n-1}, u_h^{n,j}, w) \ &= \ -\,(\tilde{\mu}_h^{n-1,j} u_h^{n,j}, w)_h, \\ &\forall\ w \in V_h,\ N_j < j \le N_a,\ 1 \le n \le N_t \end{aligned} \tag{3.89}$$

$$\begin{aligned} & u_h^{0,j} = \pi_h u(a_j, x), \quad \forall\, 1 \le j \le N_a \\ & P_h^0 = \frac{1}{2} u_h^{0,0} \tau + \sum_{j=1}^{N_a-1} u_h^{0,j} \tau \\ & u_h^{n,0} = \frac{1}{2} \tilde{\beta}_h^{n-1,0} u_h^{n,0} \tau + \sum_{j=1}^{N_a-1} \tilde{\beta}_h^{n-1,j}\, u_h^{n,j}\, \tau \\ & P_h^n = \frac{1}{2} u_h^{n,0} \tau + \sum_{j=1}^{N_a-1} u_h^{n,j} \tau, \quad \forall\, 1 \le n \le N_t \end{aligned} \tag{3.90}$$

where $\tilde{k}_h^{n-1}$ and $\tilde{\mu}_h^{n-1,j}$ are defined in the last subsection, and

$$\tilde{\mu}_h^{n-1,j}(b) = \mu(t_n, a_j, b, P_h^{n-1}), \quad \text{for} \quad \forall\ b \in \mathcal{N}_h\,.$$

In addition, since we already know the exact solution $u(t,a,x)$ of (3.85) satisfies $u(t,A_m,x)=0$, we then assume explicitly that

$$u_h^{n,N_a}=0, \qquad n=1,2,\cdots,N_t. \tag{3.91}$$

Clearly, the first two equalities (3.88) (3.89) consist of the core portion of the numerical scheme (3.88)– (3.90). In fact, for any fixed n and j, $1\le j\le N_j$ and $1\le n\le N_t$, the first equality of (3.88) is just a linear system of $|\mathcal{N}_h|$ unknowns with a diagonal coefficient matrix, which possesses a unique solution as

$$u_h^{n,j}(b)=\frac{u_h^{n-1,j-1}(b)}{1+\tau\,\tilde{\mu}_h^{n-1,j}(b)}, \qquad \text{for} \quad \forall b\in\mathcal{N}_h \tag{3.92}$$

Moreover, if let $U^{n,j}=(u_h^{n,j}(b))_{b\in\mathcal{N}_h}$ then the second equality of (3.89) can be rewritten as a linear system of $|\mathcal{N}_h|$ unknowns as follows.

$$B\,U^{n,j}=\frac{1}{\tau}M\,U^{n-1,j-1}, \quad N_j<j\le N_a,\ 1\le n\le N_t \tag{3.93}$$

where B and M are defined in last subsection. It is shown in the proof of Theorem 5 that B is a *M-Matrix* since $\mathcal{J}_h$ is weakly acute. Hence, the linear system (3.93) has a unique solution, which satisfies (3.38), that is,

$$U^{n,j}\ge 0, \ \text{ if } \ U^{n-1,j-1}\ge 0\,.$$

Thus, we in fact have shown the the following existence theorem.

THEOREM 8 *With the same assumptions as Theorem* 5, *the numerical approximate scheme* (3.88)–(3.90) *has a unique nonnegative solution.*

Moreover, we also have the following bound theorem.

THEOREM 9 *Assume that all assumptions of Theorem* 8 *hold. Let* $(u_h^{n,j},\ P_h^n)$ *be defined by the numerical scheme* (3.88) – (3.90). *There then exists a constant* C, *independent of* h *and* τ, *such that*

$$\begin{aligned} \|u_h^{n,j}\|_0 &\le C, \quad j=0,1,\cdots,N_a,\ n=1,2,\cdots,N_t \\ \|P_h^n\|_0 &\le C, \quad n=1,2,\cdots,N_t. \end{aligned}$$

Proof. From (3.92) and Theorem 8, we have that, for $1 \le j \le N_j$ and $1 \le n \le N_t$,

$$0 \le u_h^{n,j}(b) \le u_h^{n-1,j-1}(b), \quad \text{for } \forall\, b \in \mathcal{N}_h;$$

this, implies that, by a direct computation,

$$(u_h^{n,j}, u_h^{n,j})_h \le (u_h^{n-1,j-1}, u_h^{n,j})_h, \quad \forall\, 1 \le j \le N_j, \quad 1 \le n \le N_t. \tag{3.94}$$

By taking $w = u_h^{n,j}$ in (3.89), we have that, for $N_j < j \le N_a$ and $1 \le n \le N_t$,

$$\frac{1}{\tau}(u_h^{n,j} - u_h^{n-1,j-1}, u_h^{n,j})_h + \alpha_h(\tilde{k}_h^{n-1}, u_h^{n,j}, u_h^{n,j}) = -(\tilde{\mu}_h^{n-1,j}\, u_h^{n,j}, u_h^{n,j})_h.$$

This implies

$$(u_h^{n,j}, u_h^{n,j})_h \le (u_h^{n-1,j-1}, u_h^{n,j})_h, \quad \forall N_j < j \le N_j, \quad 1 \le n \le N_t. \tag{3.95}$$

Thus, combining (3.94) and (3.95),

$$(u_h^{n,j}, u_h^{n,j})_h \le (u_h^{n-1,j-1}, u_h^{n,j})_h. \tag{3.96}$$

Therefore, by an argument almost same as the proof of Theorem 5, we can obtain immediately Theorem 9.

We now consider the convergence error estimates for the numerical scheme (3.88) – (3.90). Let (u, P) solve the problem (3.85) and $(u_h^{n,j},\ P_h^n)$ solve the numerical approximate problem (3.88) – (3.90), respectively. For simplicity, except for using (3.57), we also introduce the following notations.

$$\begin{aligned} \delta^{n,j} &= u^{n,j} - u_h^{n,j} \\ \zeta^n &= P^n - P_h^n \\ \sigma^{n,j} &= \pi_h\, u^{n,j} - u_h^{n,j} \end{aligned} \tag{3.97}$$

where π_h is the standard linear interpolation operator defined in last subsection.

THEOREM 10 *With the same assumptions as Theorem 7, we then have the fol-*

lowing error estimates for the numerical approximate problem (3.88) - (3.90)

$$\|u - u_h\|_{\ell^{\infty,2}(L^2)} \leq C(\tau + h^2)$$
$$\|P - P_h\|_{\ell^2(L^2)} \leq C(\tau + h^2),$$

where the constant C *is independent of* τ *and* h *but is dependent on* u *and the given data.*

Proof. By (3.88) and Taylor's expansion, we have that, for $1 \leq j \leq N_j$, $1 \leq n \leq N_t$ and $b \in \mathcal{N}_h$,

$$\begin{aligned}
&\frac{\delta^{n,j}(b) - \delta^{n-1,j-1}(b)}{\tau} \\
&= \frac{u(t_n, a_j, b) - u(t_{n-1}, a_{j-1}, b)}{\tau} - \frac{u_h^{n,j}(b) - u_h^{n-1,j-1}(b)}{\tau} \\
&= -\mu(t_n, a_j, b, P^n(b)\,)u(t_n, a_j) + \tilde{\mu}_h^{n-1,j}\, u^{n,j} + O(\tau) \\
&= -\tilde{\mu}_h^{n-1,j}(b)\delta^{n,j}(b) + (\tilde{\mu}^{n-1,j}(b) - \mu(t_n, a_j, b, P^n(b)\,)u(t_n, a_j, b) + O(\tau) \\
&= -\tilde{\mu}_h^{n-1,j}(b)\, \delta^{n,j}(b) + C|\zeta^{n-1}(b)| + O(\tau),
\end{aligned}$$

which implies that

$$\begin{aligned}
|\delta^{n,j}(b)| &\leq (1 + \tau\, \tilde{\mu}_h^{n-1,j}(b))|\delta^{n,j}(b)| \\
&\leq |\delta^{n-1,j-1}(b)| + C\tau|\zeta^{n-1}(b)| + O(\tau^2).
\end{aligned}$$

Furthermore, it follows from trapezoidal rule that

$$\begin{aligned}|\zeta^n(b)| &= |\int_0^{A_m} u(t_n,a,b)da - \left(\frac{1}{2}u_h^{n,0}(b)\tau + \sum_{j=1}^{N_a} u^{n,j}(b)\,\tau\right)| \\ &\leq \|\delta^n(b)\|_{\ell^1} + O(\tau^2),\end{aligned}$$

where $\|\cdot\|_{\ell^1}$ is defined in the proof of Lemma 8. Therefore,

$$|\delta^{n,j}(b)| \leq |\delta^{n-1,j-1}(b)| + C\tau\|\delta^{n-1}(b)\|_{\ell^1} + C\tau^2.$$

From the definition of the linear interpolation (cf. [15]) and (3.97)

$$\begin{aligned}\delta^{n,j}(b) &= u^{n,j}(b) - u_h^{n,j}(b) \\ &= (\pi_h u^{n,j})(b) - u_h^{n,j}(b) \\ &= \sigma^{n,j}(b), \quad \text{for} \quad \forall \;\; b \in \mathcal{N}_h\end{aligned}$$

and by a direct computation, we have that

$$\|\sigma^{n,j}\|_h^2 - \|\sigma^{n-1,j-1}\|_h^2 \leq C\tau\|\sigma^n\|_{\ell^1(h)}^2 + C\tau^4\,.$$

From (3.97),

$$\|u^{n,j} - \pi_h(u^{n,j})\|_0 \leq Ch^2|u^{n,j}|_2$$

$$\delta^{n,j} = [u^{n,j} - \pi_h(u^{n,j})] + \sigma^{n,j}.$$

Hence, combining the above three inequalities together and using the triangle inequality, we obtain that

$$\begin{aligned} \|\delta^{n,j}\|_h^2 - \|\delta^{n-1,j-1}\|_h^2 &\le C\tau\|\delta^n\|^2_{\ell^1(h)} + C(h^4+\tau^4), \\ &\text{for} \quad 1 \le j \le N_j,\ 1 \le n \le N_t. \end{aligned} \tag{3.98}$$

On the other hand, from (3.57) and (3.97),

$$\delta^{n,j} = u^{n,j} - u_h^{n,j} = \eta^{n,j} + \xi^{n,j}, \tag{3.99}$$

and it follows from Lemma 10 that

$$\|\eta^{n,j}\|_0 + h|\eta^{n,j}|_1 \le Ch^2\|u^{n,j}\|_2 \tag{3.100}$$

$$\|\partial\eta^{n,j}\|_0 + h|\partial\eta^{n,j}|_1 \le Ch^2(\|u^{n,j}\|_2 + \|\partial u^{n,j}\|_2), \tag{3.101}$$

where ∂ in (3.101) is defined in Lemma 10. Thus, it follows from (3.98), (3.99), (3.100) and the triangle inequality that

$$\begin{aligned} \|\xi^{n,j}\|_h^2 - \|\xi^{n-1,j-1}\|_h^2 &\le C\tau\|\xi^n\|^2_{\ell^1(h)} + C(h^4+\tau^4), \\ &\text{for} \quad 1 \le j \le N_j,\ 1 \le n \le N_t. \end{aligned} \tag{3.102}$$

We now consider the case: $N_j < j \le N_a$ and $1 \le n \le N_t$. By a similar argument as the corresponding part of the proof for Theorem 7, we have that

$$||P^n - P_h^n||_0 \le ||\xi^n||_{\ell^1(L^2)} + Ch^2||u^{n,j}||_2 + O(\tau) \tag{3.103}$$

and

$$\begin{aligned} &||\xi^{n,j}||_h^2 - ||\xi^{n-1}||_h^2 + \frac{3k_1}{2}||\nabla\xi^{n,j}||_0^2\tau \\ &\le C\tau||\xi^{n,j}||_h^2 + C\tau||\xi^{n-1}||_{\ell^1(L^2)}^2 + C(h^4+\tau^2)\tau\,. \end{aligned}$$

Hence,

$$\begin{aligned} ||\xi^{n,j}||_h^2 - ||\xi^{n-1,j-1}||_h^2 \;\le\; & C\tau||\xi^{n,j}||_h^2 + C\tau||\xi^{n-1}||_{\ell^1(L^2)}^2 + C(h^4+\tau^2)\tau \\ & \text{for} \quad N_j < j \le N_a,\ 1 \le n \le N_t. \end{aligned}$$

So, this together with (3.102) implies that

$$\begin{aligned} ||\xi^{n,j}||_h^2 - ||\xi^{n-1,j-1}||_h^2 \;\le\; & C\tau(||\xi^{n,j}||_h^2 + ||\xi^{n-1}||_{\ell^1(L^2)}^2) + C(h^4+\tau^2) \\ & \text{for} \quad 1 \le j \le N_a,\ 1 \le n \le N_t. \end{aligned}$$

Summing it over $1 \le j \le N_a$ and using Schwarz's inequality (cf. [1, 34, 35, 106]), we then obtain that

$$\begin{aligned} &||\xi^n||_{\ell^2(h)}^2 - ||\xi^{n-1}||_{\ell^2(h)}^2 \\ &\le \tau||\xi^{n,0}||_h^2 + C\tau(||\xi^n||_{\ell^2(h)}^2 + ||\xi^{n-1}||_{\ell^2(h)}^2) + C(h^4+\tau^2)\tau. \end{aligned} \tag{3.104}$$

Observing the numerical scheme (3.27) and (3.89) - (3.90), and using a similar argument as in the proof of Theorem 7, we can also have the estimates like (3.72) and (3.75), that is,

$$\|\xi^{n,0}\|_h \le C(\|\xi^n\|_{\ell^1(h)} + \|\xi^{n-1}\|_{\ell^1(h)}) + C(h^2+\tau) \tag{3.105}$$

$$\|\xi^0\|_0 \le 2\|\xi^0\|_{\ell^2(L^2)} \le Ch^2. \tag{3.106}$$

Then, plugging (3.105) into (3.104), we have

$$(1-C\tau)\|\xi^n\|^2_{\ell^2(h)} \le (1+C\tau)\|\xi^{n-1}\|^2_{\ell^2(h)} + C(h^4+\tau^2)\tau.$$

Therefore, summing over $1 \le n \le K < N_t$ and using the Gronwall inequality (cf. [63, 90, 107, 108]), we have that, if τ and h is sufficiently small,

$$\|\xi^K\|^2_{\ell^2(h)} \le C\,\|\xi^0\|^2_{\ell^2(h)} + C\,(h^4+\tau^2)$$

this means,

$$\|\xi^K\|^2_{\ell^2(L^2)} \le C\,\|\xi^0\|^2_{\ell^2(L^2)} + C\,(h^4+\tau^2)$$

which, together with (3.105), implies

$$\|\xi\|_{\ell^{\infty,2}(L^2)} \le C(\tau+h^2). \tag{3.107}$$

Finally, using the triangle inequality, (3.107), (3.99) and (3.100), we have

$$\|u - u_h\|_{\ell^{\infty,2}(L^2)} = \|\delta\|_{\ell^{\infty,2}(L^2)} \leq \; C(\tau + h^2),$$

and plugging (3.107) into (3.103), we obtain

$$\|P - P_h\|_{\ell^2(L^2)} = \|\zeta\|_{\ell^2(L^2)} \leq \; C(\tau + h^2).$$

This completes the proof.

COROLLARY 2 *Under the same assumptions as Theorem* 10, *we then have that, for any* $j = 0, 1, \cdots, N_a$, $n = 1, 2, \cdots, N_t$,

$$\begin{aligned} \|u^{n,j} - u_h^{n,j}\|_0 \; &\leq \; C(\tau + h^2) \\ \| \, P^n - P_h^n \, \|_0 \; &\leq \; C(\tau + h^2) \end{aligned}$$

where the constant C *is independent of* τ *and* h.

Remark 3.2.3.1: Like **Remark 3.2.2.1**, it is not difficult to show from the proof for Theorem 10 that the local truncation error of numerical approximate scheme (3.88) - (3.90) has the accuracy of $O(\tau^2 + h^2)$. That is,

$$\|u^{n,j} - u_h^{n,j}\|_0 + \|P^n - P_h^n\|_0 = O(\tau^2 + h^2).$$

Remarks 3.2.3.2: Consider the model with both diffusion and advection, that is, the flux $\mathcal{D}$ in the model is defined in the following

$$\mathcal{D} = \tilde{k}\,\nabla u + \tilde{\mathbf{q}}\,u\,.$$

By a similar argument as **Remark 3.2.2.3**, we can show that Theorem 8, Theorem 9, Theorem 10 and Corollary 2 are still true for the model with both diffusion and advection theoretically if the time-age step τ, advection term $\mathbf{q}$ and the mortality μ are "*good*" enough to make the approximate bilinear form (1.14) coercive of we apply the special treatment to the model, for example, taking a very small *time-age* step size τ or taking the transformation as in **Remark 2.3.1** and **Remark 2.3.2** to change the original model to a new one whose approximate bilinear form (1.14) is coercive. However, as the arguments in **Remark 3.2.2.4**, we usually apply a *upwind* scheme, $R_h(\mathbf{q}\,u,\ \nabla v)$, to replace $(\mathbf{q}\,u,\ \nabla v)_h$ of the numerical approximate scheme (3.88) - (3.90). We will analyze this *upwind* scheme later.

3.3 Numerical Scheme for Mathematical Models of Individual-Based Populations

This section develops and analyzes a numerical approximate scheme for the mathematical models for individual-based populations in a heterogeneous spatial chemical toxicant environment as proposed in the previous chapters. The mathematical models include an initial value ordinary differential system problem for the individual model and a nonlocal initial-boundary value nonlinear partial differential problem with discontinuous coefficients for individual-based population dynamics including diffusion and advection. The numerical approximation scheme is based on the three basic techniques of the mathematical analyses in Chapter 2, which are localization, unstructuralization for physiological structures and linearization. In order to develop and analyze the numerical scheme, we apply the related numerical schemes and their analyses for the initial value ordinary differential system and the auxiliary age structured population problems discussed in the last two sections. For the ordinary differential system problem of the individual model, we simply apply the implicit Runge-Kutta method of Section 2 of this Chapter. However, the numerical scheme is much more complicated for the partial differential problem of the population dynamics model. The basic idea is to apply a characteristic finite difference discretization for time-age domain $(0,T] \times [0,A_m]$ and a finite element discretization for spatial domain Ω. The discussions have shown that the numerical scheme guarantees a biological approximate solution and has a good approximate error accuracy. We will use the same partitions for $(0,T] \times [0,A_m]$ and Ω as in the last section. Also, we will use the other notations defined in the last subsection.

For convenience, we would like rewrite the mathematical model for individual-based fish population dynamics as follows.

Individual Model:

$$\begin{aligned} \frac{dm_L}{da} &\equiv g_L = G_L - F_L, \\ \frac{dm_S}{da} &\equiv g_S = G_S - F_S \end{aligned} \tag{3.108}$$

$$\begin{aligned} m_L|_{a=0} &= m_{L_0} \\ m_S|_{a=0} &= m_{S_0} \end{aligned} \tag{3.109}$$

Population Dynamic Model:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial a} + \frac{\partial(\rho\, g_L)}{\partial m_L} + \frac{\partial(\rho\, g_S)}{\partial m_S} = -\mu\rho \qquad \text{for } t \in (0,T], a \in (0,J], x \in \Omega \tag{3.110}$$

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial a} + \frac{\partial(\rho\, g_L)}{\partial m_L} + \frac{\partial(\rho\, g_S)}{\partial m_S} - \nabla \cdot (k\nabla\rho) = -\mu\rho \qquad \text{for } t \in (0,T], a \in (J,A], x \in \Omega \tag{3.111}$$

$$\begin{aligned} & k\frac{\partial \rho}{\partial \nu} = 0 \quad \text{or} \quad \rho = 0, \quad x \in \partial\Omega \\ & \rho(0, a, m_L, m_S, x) = \rho_0(a, m_L, m_S, x) \\ & \rho(t, 0, m_{0L}, m_{0S}, x) = \int_0^{A_m}\int_0^{\infty}\int_0^{\infty} \beta\rho(t, a, m_L, m_S, x)\, da\, dm_L\, dm_S \end{aligned} \tag{3.112}$$

For the case with chemical toxic ant effects, (3.108) should be replaced by

Individual Model with Toxicant Effects:

$$\begin{aligned} \frac{dm_L}{da} &\equiv g_L = \chi G_L - F_L \\ \frac{dm_S}{da} &\equiv g_S = \chi G_S - F_S \end{aligned} \tag{3.113}$$

$$\begin{aligned} m_L|_{a=0} &= m_{L_0} \\ m_S|_{a=0} &= m_{S_0} \end{aligned} \tag{3.114}$$

$$\begin{aligned} \frac{dB_T}{da} &\equiv g_c = sk_w C_w + C_F F - \frac{B_T}{W_T BCF}(sk_w + Ek_E) \\ B_T|_{a=0} &= B_{T_0} \end{aligned} \tag{3.115}$$

To apply the finite element method for (3.111), we first have to introduce its weak formulation as follows.

$$\begin{aligned} &(\frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial a} + \frac{\partial \rho}{\partial m_L}\, g_L + \frac{\partial \rho}{\partial m_S}\, g_S,\ w)\ +\ \alpha(k,\ \rho,\ w) \\ &\quad + ((\mu + \frac{\partial g_L}{\partial m_L} + \frac{\partial g_S}{\partial m_S})\rho, w) = 0, \quad \forall\ \ w \in H^1(\Omega). \end{aligned} \tag{3.116}$$

Before constructing a numerical approximate scheme for the above mathematical model problems, we need to rewrite the local problems mathematically. As in their mathematical analyses and discussions in Chapter 2, we suppose that, for fish, n tasks (feeding, reproduction, movement, etc) are accomplished sequentially (cf. [54]). Thus, based on the above biological assumption, we can localize, unstructuralize and linearize the mathematical model problems in a small time interval. In particular, we may separately solve the individual model and population dynamic model in a local level (i.e. in a small time interval). Therefore, the numerical scheme allows us to solve the individual model and population model sequentially and split them at every single time step. More precisely, at every single time step, we first solve the individual model independently, plug the solution of the individual model at this time step, which is just obtained, into the population model and then solve the population model at this time step.

For every time step $[t_{i-1}, t_i]$, we suppose that

$$\begin{cases} m_L &= m_L(a, t_i, \cdots) \\ m_S &= m_S(a, t_i, \cdots) \end{cases}$$

is the solution of the individual model in the time step $[t_{i-1}, t_i]$, and let

$$\tilde{\rho}(t, a, x) = \rho(t, a, m_L(a, t_i, \cdots), m_S(a, t_i, \cdots), x)\,. \tag{3.117}$$

Therefore, the population model (3.110) (3.111) in $[t_{i-1}, t_i]$ can be modified as

$$\frac{\partial \tilde{\rho}}{\partial t} + \frac{\partial \tilde{\rho}}{\partial a} = -(\mu + \frac{\partial g_L}{\partial m_L} + \frac{\partial g_S}{\partial m_S})\tilde{\rho}, \qquad t \in [t_{i-1}, t_i] \tag{3.118}$$

$$\frac{\partial\tilde{\rho}}{\partial t}+\frac{\partial\tilde{\rho}}{\partial a}+\nabla(k\ \nabla\tilde{\rho}) = -(\mu+\frac{\partial g_L}{\partial m_L}+\frac{\partial g_S}{\partial m_S})\tilde{\rho}, \quad t\in[t_{i-1},t_i]\,. \tag{3.119}$$

moreover, the weak formulation (3.116) can be modified as

$$\begin{aligned}(\tilde{\partial}_\tau\tilde{\rho},w)+\alpha(k,\tilde{\rho},w) &= -((\mu+\frac{\partial g_L}{\partial m_L}+\frac{\partial g_S}{\partial m_S})\tilde{\rho},\ w), \\ &\qquad \forall\ \ w\in V,\ \ t\in[t_{i-1},t_i]\end{aligned} \tag{3.120}$$

Thus, using the related algorithms and notations of last two section of this Chapter, we are now ready to construct a numerical scheme for the individual-based fish population models (3.113) - (3.116). Like the mathematical model problem for individual-based fish populations, the numerical scheme also consists two parts. The numerical discretization for the individual model, either a single individual model if without chemical toxicant effects or an individual model together with a uptake toxicant equation if with chemical toxicant effects is combined with the numerical discretization for the population dynamic model.

Numerical Discretization for Individual Model:

$$\begin{cases} m_L^j &= m_L^{j-1}+g_L(a_j+\frac{1}{2}\tau,\frac{1}{2}(m_L^{j-1}+m_L^j),\frac{1}{2}(m_S^{j-1}+m_S^j),b) \\ m_S^j &= m_S^{j-1}+g_L(a_j+\frac{1}{2}\tau,\frac{1}{2}(m_L^{j-1}+m_L^j),\frac{1}{2}(m_S^{j-1}+m_S^j),b), \end{cases}$$

$$\text{for}\quad\forall\ \ b\in\mathcal{N}_h,\ i=1,2,\cdots,N_a \tag{3.121}$$

$$m_L^0 = m_{L_0}(b),\quad \text{(given)}\quad \text{for}\quad \forall\ \ b\in\mathcal{N}_h$$

$$m_S^0 = m_{S_0}(b),\quad \text{(given)}\quad \text{for}\quad \forall\ \ b\in\mathcal{N}_h$$

Numerical Discretization for Population Model:

For $1 \le j \le N_a$ and $1 \le n \le N_t$, seeking $\rho_h^{n,j} = \sum_{b \in \mathcal{N}_h} \rho_h^{n,j}(b)\varphi_b \in V_h$, such that

$$\begin{aligned} \frac{\rho_h^{n,j}(b) - \rho_h^{n-1,j-1}(b)}{\tau} &= -\tilde{\mu}_h^{n-1,j}(b)\, \rho_h^{n,j}(b), \quad \forall\, b \in \mathcal{N}_h \\ & \quad 1 \le j \le N_j,\ 1 \le n \le N_t \end{aligned} \tag{3.122}$$

$$\begin{aligned} (\tilde{\partial}_\tau \rho_h^{n,j}, w)_h + \alpha_h(\tilde{k}_h^{n-1}, \rho_h^{n,j}, w) &= -(\tilde{\mu}_h^{n-1,j} \rho_h^{n,j}, w)_h, \quad \forall\, w \in V_h \\ & \quad N_j < j \le N_a,\ 1 \le n \le N_t \end{aligned} \tag{3.123}$$

$$\begin{aligned} &\rho_h^{0,j} = \pi_h \rho(a_j, m_{L_0}, m_{S_0}, x), \quad \forall\, 1 \le j \le N_a \\ &P_h^0 = \frac{1}{2}\rho_h^{0,0}\tau + \sum_{j=1}^{Na-1} \rho_h^{0,j}\tau \\ &\rho_h^{n,0} = \frac{1}{2}\tilde{\beta}_h^{n-1,0}\rho_h^{n,0}\tau + \sum_{j=1}^{Na-1} \tilde{\beta}_h^{n-1,j}\rho_h^{n,j}\tau \\ &P_h^n = \frac{1}{2}\rho_h^{n,0}\tau + \sum_{j=1}^{Na-1} \rho_h^{n,j}\tau, \quad \forall\, 1 \le n \le N_t \end{aligned} \tag{3.124}$$

where $\tilde{k}_h^{n-1}$ is defined in (3.28) of last Section and

$$\begin{aligned} \tilde{\mu}_h^{n-1,j}(b) &= \mu(t_n, a_j, m_L^j, m_S^j, b, P_h^{n-1}) \\ &\quad + \frac{g_L}{m_L}\Big|_{(t_n,a_j,m_L^j,m_S^j,b)} + \frac{g_S}{m_S}\Big|_{(t_n,a_j,m_L^j,m_S^j,b)} \\ \tilde{\beta}_h^{n-1,j}(b) &= \beta(t_n, a_j, m_L^j, m_S^j, b, P_h^{n-1}). \end{aligned} \tag{3.125}$$

In addition, since we already know the exact solution ρ of (3.82) – (3.84) satisfies

$\rho(t, A_m, m_L, m_S, x) = 0$, we then assume explicitly that

$$\rho_h^{n,N_a} = 0, \quad \text{for} \quad 1 \leq n \leq N_t \tag{3.126}$$

If the problem also includes advection, we need apply a *upwind scheme* to modify the approximate bilinear form $\alpha_h(\cdots)$ as in **Remark3.2.2.4**. On the other hand, if there are chemical effects for fish, the numerical scheme for individual model (3.121) needs to be replaced by the following numerical discretization for *Individual Model with Toxicant Effects* (3.113) - (3.115), that is, a modified individual growth model together with a chemical toxicant uptake equation.

Numerical Discretization for Individual Model with Toxicant Effects:

$$\left\{\begin{array}{lcl} m_L^j & = & m_L^{j-1} + g_L^j(a_j + \frac{1}{2}\tau, \frac{1}{2}(m_S^{j-1} + m_S^j), \frac{1}{2}(m_L^{j-1} + m_L^j), b) \\ m_S^j & = & m_S^{j-1} + g_S^j(a_j + \frac{1}{2}\tau, \frac{1}{2}(m_S^{j-1} + m_S^j), \frac{1}{2}(m_L^{j-1} + m_L^j), b), \end{array}\right.$$

$$\text{for} \quad \forall \ b \in \mathcal{N}_h, \ i = 1, 2, \cdots, N_a \tag{3.127}$$

$$m_L^0 = m_{L_0}(b), \quad \text{for} \quad \forall \ b \in \mathcal{N}_h$$

$$m_S^0 = m_{S_0}(b), \quad \text{for} \quad \forall \ b \in \mathcal{N}_h$$

$$B_T^j = B_T^{j-1} + g_c(a_j + \frac{1}{2}\tau, \frac{1}{2}(B_T^{j-1} + B_T^j)),$$

$$\text{for} \quad \forall \ b \in \mathcal{N}_h, \ i = 1, 2, \cdots, N_a \tag{3.128}$$

$$B_T^0 = B_{T_0}(b), \quad \text{for} \quad \forall \ b \in \mathcal{N}_h$$

where

$$\begin{aligned}
g_L^j &= \tilde{\chi}^{j-1}(G_L - F_L)\big|_{(a_j+\frac{1}{2}\tau, \frac{1}{2}(m_L^{j-1}+m_L^j), \frac{1}{2}(m_L^{j-1}+m_L^j), b)} \\
g_S^j &= \tilde{\chi}^{j-1}(G_S - F_S)\big|_{(a_j+\frac{1}{2}\tau, \frac{1}{2}(m_L^{j-1}+m_L^j), \frac{1}{2}(m_L^{j-1}+m_L^j), b)} \\
\tilde{\chi}^{j-1} &= \chi(B_T^{j-1})
\end{aligned}$$

and g_c stands for the right hand side term of the chemical uptake equation (3.115). Furthermore, we would like to mention that, in numerical computation experiments, we may plug back B_T^j to replace the old B_T^{j-1} into $\tilde{\chi}^{j-1}$ and then solve (3.127) - (3.128) one or more times as in a Predictor-Corrector Method in order to increase the accuracy (cf. [76, 88]).

Clearly, (3.122) (3.123) is the key portion. In particular, (3.123) is indeed an ill-conditioned linear system as in (3.93), i.e.,

$$\begin{aligned}
(\frac{1}{\tau}\, M + A + D)\, U^{n,j} &= \frac{1}{\tau} M\; U^{n-1,j-1}, \\
&\quad \text{for} \quad N_j < j \leq N_a,\ 1 \leq n \leq N_t
\end{aligned} \tag{3.129}$$

where $B \equiv \frac{1}{\tau}\, M + A + D$ is defined as in (3.93). The linear system (3.129) is not easily solved. We will give a parallel method to solve this kind of linear system in the last section of this chapter.

Notice that the definition of $\tilde{\mu}_h^{n-1,j}(b)$ in (3.122) and (3.123) is different from that in (3.88) and (3.89). However, if τ is sufficiently small, we still have that the properties: $1 + \tau\, \tilde{\mu}_h^{n-1,j}(b) > 0$ and B is a *M-Matrix*. So, combining with the unique existence of numerical scheme of Individual Model (3.108) - (3.109) or Individual Model with Toxicant Effects (3.113) - (3.115), we have the following proposition by similar arguments as the proof of Theorem 3 in Chapter 2. This proposition guarantees the numerical scheme always produces a biologically reasonable approximate solution.

PROPOSITION 3 *If* $\tau > 0$ *is sufficiently small, then the numerical scheme* (3.121) *(or* (3.127) - (3.128) *if there are toxicant effects) and* (3.122) - (3.124) *has a unique solution. In particular, the solution of the numerical discretization for the population model is always nonnegative.*

We are now discuss the convergence error estimates for the numerical schemes. Considering the numerical discretization for individual model (3.121) and (3.127) (3.128), we have from Lemma 4 that both m_L^j and m_S^j have at least the local truncation error accuracy estimate with order of $O(\tau^2)$. Thus, by a direct computation about g_L, $\frac{\partial g_L}{\partial m_L}$ and g_S, $\frac{\partial g_S}{\partial m_S}$, we obtain from (3.125) that k_h^{n-1} , $\tilde{\mu}_h^{n-1,j}$ and $\tilde{\beta}_h^{n-1,j}$ have error estimate $O(\tau^2 + \|P^{n-1} - P_h^{n-1}\|_0)$; that is,

$$\begin{aligned}
&\| k(t_n, x, P^n) - k_h^{n-1}(x) \|_0 \;\le\; C\|P^n - P_h^{n-1}\|_0 + O(\tau^2),\\
&\|\mu(t_n, a_j, m_L|_{(a_j,\cdots)}, m_S|_{(a_j,\cdots)}, x, P^n) + \frac{\partial g_L}{m_L}|_{(a_j,\cdots)} + \frac{\partial g_S}{m_S}|_{(a_j,\cdots)} - \tilde{\mu}^{n-1,j}(x) \|_0\\
&\quad \le\; C\|P^n - P_h^{n-1}\|_0 + O(\tau^2),\\
&\|\beta(t_n, a_j, m_L|_{(a_j,\cdots)}, m_S|_{(a_j,\cdots)}, x, P^n) \;-\; \tilde{\beta}^{n-1,j}(x) \|_0\\
&\quad \le\; C\|P^n - P_h^{n-1}\|_0 + O(\tau^2),
\end{aligned}$$

where we have used the local truncation error estimate of the numerical approximate solutions of the fish individual model

$$|m_L^j - m_L(a_j, \cdots)| + |m_S^j - m_S(a_j, \cdots)| = O(\tau^2).$$

Then, observing the related discussions of last section of this chapter, we could find the similar arguments may apply to the numerical discretization (3.122) – (3.124). So, we may have that

PROPOSITION 4 *The computational model for individual-based fish populations* (3.121) (*or*(3.127) (3.128)) *and* (3.122) – (3.124) *have the local truncation error estimate with order of* $O(\tau^2 + h^2)$.

Finally, we give some examples for k, μ and β and their approximations k_h^{n-1}, $\mu_h^{n-1,j}$ and $\beta_h^{n-1,j}$, which will be applied in the computational experiments of Chapter 4 and Chapter 5. We only consider two simple diffusions (cf. [29], [93], [96]). One is the purely random walk dispersal, that is $k = constant$. Clearly, we then take $k_h^{n-1} = constant$. The other is the random plus density-dependent dispersal, for instance,

$$k = 1 + \kappa_p \hat{P}.$$

where κ_p is a constant and $\hat{P}$ stands for total number of all adult fish, that is,

$$\hat{P} = \int_J^{A_m} \rho \, da.$$

For this case, we can take that

$$k_h^{n-1} = 1 + P_h^{n-1}.$$

Therefore, it is easy to see that the above k_h^{n-1}'s satisfy the approximate estimates we need. We now consider the mortality function μ. For the fish at a location x and time t, we assume that (cf. [47, 82])

$$\mu = \mu_a + \mu_w + \mu_y + \mu_d,$$

where μ_a, μ_w, μ_y and μ_d will be defined next. The age-dependent mortality, μ_a, is assessed uniformly along fish born at the same time, which is defined as follows.

$$\mu_a = \begin{cases} \kappa_a \ , & \text{if} \quad 0 \le a < A_m \\ \infty \ , & \text{if} \quad a \ge A_{max} \end{cases} \tag{3.130}$$

where κ_a is the mortality rate of individuals of age a. The weight-dependent mortality, μ_w, viewed as possibly caused by predation and determined by the weight of the individual, is defined as $\mu_w = \gamma_w \cdot \mu_{1w} = \gamma_w \cdot \mu_{1w}(W)$, where γ_w is a constant parameter, W is the weight of the individual and

$$\mu_{1w} = \begin{cases} V_0, & \text{if } \; W = 0 \\ V_C, & \text{if } \; W_1 \leq W \leq W_2 \\ V_F, & \text{if } \; W = W_3 \\ \text{continuous and linear,} & \text{elsewhere.} \end{cases} \tag{3.131}$$

The mortality to the young of the year, μ_y, is assessed uniformly across the population with age in the embryonic stage $[0,\ J]$. The mortality might be caused by predation or overcrowding. The specific forms of density-dependent mortality are defined as

$$\mu_y = \begin{cases} \mu_J \dfrac{P_J}{P_c}\ , & \text{if } \; 0 < P_J < P_c \; \text{ and } \; a \in [0,\ J] \\ \mu_J\ , & \text{if } \; P_J \geq P_c \; \text{ and } \; a \in [0,\ J] \end{cases} \tag{3.132}$$

where P_J is total population with age in the interval $[0,\ J]$, μ_J is a constant rate of mortality and P_c is the largest number of juveniles the environment can support. The density-dependent mortality, μ_d, is defined as

$$\mu_d = \begin{cases} D_M, & \text{if } \; 0 \leq P_B \leq P_T \\ D_0, & \text{if } \; P_B = P_0 \\ D_C, & \text{if } \; P_B \geq P_C \\ \text{continuous and linear,} & \text{elsewhere} \end{cases} \tag{3.133}$$

where P_B is the total population biomass and all the others are constant parameters that can be found in [47, 82, 87]. Notice that the weight, W, is a linear function of $(m_L + m_S)$. Thus, μ can be rewritten as

$$\mu = \mu(t, a, m_L, m_S, x, P) .$$

In particular, μ has a piecewise linear relationship for a, m_L, m_S and P over age interval $[0, A_m]$, respectively. Therefore, if we choose $\mu_h^{n-1,j}$ as in (3.125), we can show easily that the $\mu_h^{n-1,j}$ satisfy the approximate estimates we need. From the descriptions of the reproduction processes in Section 1.2 of Chapter 1, we can see that β can be expressed as the following form

$$\beta = \beta_a \, \beta_t \, \beta_0$$

where

$$\beta_a = \begin{cases} 0, & \text{if } \ 0 \le a < J \\ > 0, & \text{if } \ a \ge J \end{cases}$$

$$\beta_t = \begin{cases} > 0, & \text{if } \ t \text{ in the reproduction window} \\ 0, & \text{elsewhere} \end{cases}$$

and

$$\beta_0 = \beta_0(m_L, m_S, x, P),$$

in particular, β_0 is linear with respect to P and continuous with respect to m_L and m_S. Hence, if we choose $\beta_h^{n-1,j}$ as in (3.125), then we can have proved that $\beta_h^{n-1,j}$ satisfy the approximate estimates we need.

Remark 3.3.1: Like **Remark 3.2.2.3**, **Remark 3.2.2.4** and **Remark 3.2.3.2**, we could extend the analyses and discussions of this section to the population dynamic model with both diffusion and advection, that is, $k\nabla u$ is replaced by $k\nabla u - \mathbf{q}\,u$. The approximation of $\mathbf{q}$ is defined as

$$\mathbf{q}_h^{n-1,j} = \mathbf{q}(t_n, a_j, m_L^j, m_S^j, x, P_h^{n-1}) .$$

In our numerical experiments, we have considered the advection movements because of the heterogenity of resource (food) or/and chemical toxicant by using a *upwind* numerical scheme. For example, $\mathbf{q}$ is defined in (4.5) of Chapter 4 or/and (5.10). It will shown that we can define $\mathbf{q}_h^{n-1,j}$ with a good approximate error such that the error estimates of whole approximation solutions aren't decreased.

3.4 Computational Model and Algorithm Aspects

This section discusses a computational model and its related algorithm aspects for numerically simulating the individual-based fish population in a spatially heterogeneous chemical toxicant environment. The computational model is based on the mathematical model of individual-based fish population developed in Chapter

2 and the numerical approximation schemes developed in the previous sections of this chapter. The mathematical model mainly consists of a ordinary differential system of inidividual model and a nonlocal nonlinear degenerate parabolic partial differential problem of population dynamic model. We construct the numerical simulation for individual growth by using the implicit Runge-Kutta numerical scheme for the initial value ordinary differential system problem of individual model. We construct the numerical simulation for the variation of fish population distribution based on the numerical scheme for individual-based population dynamics, which is a combination of a characteristics finite difference discretization and a linear finite element discretization with numerical integration and upwind scheme modifications.

As we all know, the advantage of individual-based mathematical and computational population models is to track individuals and their effects on population or higher levels. However, most of time, there are too many individuals in a population, so it is impossible to track every individual of the population in a practical computation. In view of a common sense in biology, the individuals with the same age and same/similar physiological characteristics are assumed to have same/similar responses on the same environment. Therefore, for a non-spatial individual-based population model, we, indeed, track each cohort, a group of individuals with same age and physiological characteristics, in the computational model (cf. [43, 44, 45, 49]). Moreover, this strategy can even work to a individual-based population model with a pure advection (cf. [50, 82, 83]). Unfortunately, this kind of cohort might be broken and split due to diffusion. Thus, the technique based on cohorts cannot be extended to the computational model for individual-based population model with movements including diffusion. Noting the fact that the individuals with same age always have the same age, we try to track *Age-Group*, a group of individuals with same age, instead of the *cohort*. We also introduce *growth-pattern* (or called *q-cohort*) into *Age-Group*. We divide an *Age-Group* into several different q-cohorts (but not too many q-cohorts). The physiological characteristics of individuals in the same q-cohort might not be the same but must be close such that these individuals can have similar responses to the same environment. In a single age-time step of the computation, the q-cohort works similarily to the cohort in a nonspatial model, that means, we calculate the final values of this step by the numerical schemes of individual model and individual-based population dynamics developed in the last section. But, when we make the transition for the current step to the next step, we must reconstruct the new q-cohorts and initial values for the next step because the old q-cohorts have already split. Thus, We can develop a computational model for individual-based population model with diffusion and advection by using the technique of tracking *Age-Group* and constructing/reconstructing q-cohorts. Therefore, incorporating the environmental variable effects and birth process, we then develop a computational model for simulating individual-based populations with environmental effects in a spatially heterogeneous chemical toxicant environment as described in a flow chart Figure 5.

Just like a cohort in a non-spatial model, we simply use an array structure for a q-cohort, each of whose array elements stores a physiological characteristic value or age. Also, we use a double linked list of q-cohort to describe the heterogeneities of individuals of the same *Age-Group* in a small spatial area (representing by a nodal point) at a special time (see Figure 6). We define a structure for an *Age-Group*. The data field of the *Age-Group* structure is an array of pointers. Each of those pointers points to the head of a double linked list of q-cohort (see Figure 7). Therefore, an *Age-Group* structure gives the distribution of the population of this *Age-Group* in spatial, age, and other physiological variables. Finally, we apply a *Dequeue* of *Age-Group* nodes to describe the distributions of the whole population, its age and its other physiological characteristics, such as lipid, protein. This *Dequeue* is described in Figure 7.

The programming code is based on the above data structures and the flow chart of computational model (see Figure 5). We give the pseudo-codes as follows.

Pseudo-code Algorithm

- Main loops
    1. Time loop
    2. Traverse the *Dequeue* of *Age-Group* from the top to base

    - if $age < J$, i.e. embryonic stage
    - if $age \geq J$, i.e. older life stage

3. Traverse the pointer array in the *Age-Group* node (loop for spatial nodal points)
4. Traverse the double linked list of q-cohort

- Embryonic stage
  - Traverse the spatial nodal points
  - Traverse the double linked list of q-cohort
  - solve the individual model (environmental & toxicant effects)
  - solve the population model (without movements)
- The older life stage
  - Traverse the spatial nodal points
  - Traverse the double linked list of q-cohort
  - Solve the individual model (environmental & toxicant effects)
  - Solve the population model with movements
  - Check birth (environmental effects)

Solve the population model with diffusion and advection

- For every q-cohort
    - Determine its maximum moving domain (pursuit and advection speed).
    - Build the linear system of approximate problem over maximum moving domain.
    - Solve the linear system
    - Store the solution value in a temporal buff.
- Construct a new double-linked list of q-cohort by data of the temporal buff.
- Replace the old double linked list of q-cohort by new one
- Update the *Age-Group*
- Release the memory of the old double-linked list of q-cohort.

3.5 A Parallel Procedure for the Linear Systems

It is easy to see that, at each time-age step, the most important key portion for our numerical schemes of the population models, for example, (3.122) - (3.124), is a linear system, which is defined as follows.

$$\left(\frac{1}{\tau}M + A + D\right)U = F \tag{3.134}$$

where $M,\ A,\ D$ is defined in (3.33) at previous sections and F is a vector. From [3, 23, 30, 36, 106], the linear system (3.134) usually is a ill-conditioned linear system, that is, the condition number of B is large. In fact, it is not hard to show that the condition number estimate of the coefficient matrix $B = \frac{1}{\tau} M + A + D$ is $O(1 + \tau\, h^{-2})$ for 2-*dimensional* domain. Thus, the linear system (3.134) is not easy to be solved by either a direct method or an iterative method since it is usually large scale, especially for higher dimension domain Ω. Therefore, it is also an interesting project to develop a good procedure for the linear system (3.134). In this section, we have developed a parallel procedure, which is a combination of the iterative method and the direct method, to solve such a linear system based on the technique of domain decomposition (cf. [23, 24, 25, 85, 106]). In fact, this parallel procedure can be regarded as a bridge connecting a direct method and an iterative method based on the parallel algorithm view point (cf. [23, 24]). There are two motivations that led us to propose this parallel procedure here. One is that we hope this parallel procedure can help to implement our numerical scheme for those population dynamic problems which cannot be implemented because its core portion, a large scale linear system, cannot be solved by the usual numerical solver. The other is that this parallel procedure is very efficient for the discrete problems of parabolic type partial different problems, like (3.134).

It is not hard to check that the linear system (3.134) is indeed the finite element equation of the following elliptic partial differential problem.

$$\begin{aligned} &-\nabla \cdot (k\nabla u) + \mu\, u + \frac{1}{\tau}\, u = f \quad \text{in} \quad \Omega \\ &k\frac{\partial u}{\partial \nu} = 0 \quad or \quad u = 0 \quad \text{on} \quad \partial\Omega \end{aligned} \tag{3.135}$$

Moreover, it is easy to see that the elliptic partial differential problem (3.135) can be obtained from the individual-based population model (3.111) after localization, unstructuralization of physiological structures and a characteristic finite difference discretization in the time-age domain. It also can be obtained from auxiliary age structured population problem (II) (or (III)) by using a characteristic finite difference discretization of the time-age domain. Its weak formulation is formulated by seeking $u \in V$, such that

$$\alpha_\Omega(u,\ w) \ = \ (f,\ w)_\Omega, \qquad \text{for} \quad \forall\ w\ \in\ V \tag{3.136}$$

where $(\cdot,\ \cdot)_\Omega$ is the inner product of $L^2(\Omega)$, i.e., the previous $(\cdot,\ \cdot)$ and

$$\begin{aligned} \alpha_\Omega(v,\ w) \ &= \ \alpha(k,\ v,\ w) + (\mu\, v,\ w)_\Omega + (\frac{1}{\tau}\, v,\ w)_\Omega \\ &= \int_\Omega (\, k\, \nabla v \cdot \nabla w \ + \ \mu\, v\, w + \frac{1}{\tau}\, v\, w\,) dx \end{aligned} \tag{3.137}$$

Furthermore, its finite element approximate problem is to seek $u_h \in V_h$, such that

$$\alpha_\Omega^h(u_h,\ w) \ = \ (f,\ w)_\Omega \qquad \text{for} \quad \forall\ w \in V_h \tag{3.138}$$

where

$$\alpha_\Omega^h(v,\ w) = (\,k\,\nabla v,\ \nabla w)_h + (\mu\, v,\ w)_h + \frac{1}{\tau}(v,\ w)_h. \tag{3.139}$$

Therefore, let M, D and A be defined in (3.33), and

$$u_h = \sum_{b\in\mathcal{N}_h} u_h(b)\,\varphi_b, \qquad U = (u_h(b)\,)_{b\in\mathcal{N}_h}, \quad F = (\,(f,\varphi_b)_\Omega)_{b\in\mathcal{N}_h},$$

then, the finite element problem (3.138) can be exactly rewritten as the linear system (3.134).

To develop our parallel procedure for the finite element problem (3.138), we first need to introduce a non-overlapping decomposition for the domain Ω, which has to be aligned with the triangulation $\mathcal{J}_h$, that means, each subdomain has to be a block of elements of $\mathcal{J}_h$. We consider a non-overlapping decomposition of the domain Ω into arbitrary number m disjoint subdomains Ω_i $(i = 1, 2, \cdots, m)$, where Ω_i is a block of elements of $\mathcal{J}_h$; that is, we assume that Ω_i $(i = 1, 2, \cdots, m)$ is a block of of elements of $\mathcal{J}_h$ and satisfies

$$\begin{aligned}
\overline{\Omega} &= \overline{\Omega}_1 \cup \overline{\Omega}_2 \cup \cdots \cup \overline{\Omega}_m \\
&= \Omega_1 \cup \Omega_2 \cup \cdots \cup \Omega_m \cup \Sigma \cup \Gamma, && (3.140) \\
\Sigma &= \bigcup_{1\le i\ne j\le m} \gamma_{ij}, \qquad \gamma_{ij} \;=\; \partial\Omega_i \cap \partial\Omega_j, && (3.141) \\
\Gamma &= \bigcup_{i=1}^{m} \Gamma_i \;\equiv\; \partial\Omega \quad \Gamma_i \;=\; \partial\Omega_i \cap \partial\Omega. && (3.142)
\end{aligned}$$

We now define our parallel algorithm as follows.

Algorithm

(i) Given $g_{ij}^0 \in V_h|_{\gamma_{ij}}$, $(i \neq j, i, j = 1, 2, \cdots, m)$, arbitrarily;

(ii) recursively compute $u_i^n \in V_h|_{\Omega_i}$, $(i = 1, \cdots, m)$ by solving the following subproblems in parallel: find $u_i^n \in V_h|_{\Omega_i}$, such that

$$\begin{aligned} \alpha_{\Omega_i}^h(u_i^n,\ v) \ &+ \sum_{1 \leq j \neq i \leq m} \lambda_{ij} \int_{\gamma_{ij}}^{*} u_i^n\, v\, ds = (f,\ v)_{\Omega_i} \\ &+ \sum_{1 \leq j \neq i \leq m} \int_{\gamma_{ij}}^{*} g_{ij}^n\, v\, ds, \qquad \forall\, v \in V_h|_{\Omega_i}, \qquad (3.143) \end{aligned}$$

(iii) update data of the transmission condition on the interfaces

$$g_{ij}^{n+1}(b) = 2\lambda_{ij}\, u_j^n(b) - g_{ji}^n(b),\ \forall\, b \in \mathcal{N}_h \cap \gamma_{ij},\ \ 1 \leq i \neq j \leq m, \qquad (3.144)$$

where the constant parameters $\lambda_{ij} = \lambda_{ji} > 0$, $\alpha_{\Omega_i}(\cdot,\ \cdot)$ and $(\cdot,\ \cdot)_{\Omega_i}$ are understood as in (3.136) and (3.137). Also,

$$\int_{\gamma_{ij}}^{*} \Psi ds \ = \sum_{e_f \subset \gamma_{ij}} \int_{e_f}^{*} \Psi\, ds \ = \sum_{e_f \subset \gamma_{ij}} \frac{meas(e_f)}{\mathbf{n}} \sum_{b_{ef} \in e_f} \Psi(b_{ef}) \qquad (3.145)$$

where $\mathbf{n}$ is the dimension number of Ω, e_f is a face of an element e of $\mathcal{J}_h$, b_{ef} is a nodal point (vertex for conforming linear finite element) on the face e_f and $meas(e_f)$ is the ($\mathbf{n}$-1)-*dimension* measure of e_f, moreover, we assume that the above integral is always 0 if $meas(\gamma_{ij}) = 0$.

Clearly, the *Algorithm* is a parallel algorithm, which can be implemented on massive parallel machines naturally and easily while assigning each subdomain to its own processor. Moreover, if we suppose that each subproblem in (ii) of the *Algorithm* is solved exactly by a direct method, then, the *Algorithm* is just a direct method if there is only one subdomain (i.e., we have not decomposed the original domain), while the *Algorithm* may be regarded as an iterative method in the usual sense if each individual element is chosen as a subdomain. Therefore, the *Algorithm* might be thought as a bridge connecting between the direct method and iterative method from the view point of a parallel algorithm (cf. [23, 24, 30, 110, 118]). This also means that, while using this method to solve a linear system, we might take advantage of both the direct and iterative method by choosing the subdomains properly.

We are going to use an energy estimate technique to prove the convergence of the parallel *Algorithm* (cf. [15, 22, 35]). In the proof, we follow the basic idea of [23, 85], which has been applied to discuss the corresponding parallel procedure for a partial differential equation continuous problem. Like [24] which considers the nonconforming linear finite element problem (cf. [21, 18]), we first need to give a splitting subproblem form for the conforming linear finite element problem (3.138) based on the nonoverlapping domain decomposition (3.140) – (3.142).

LEMMA 11 *Let* $u \in V_h$ *be the solution of the problem* (3.138). *Then there exist*

$$g_{ij} \in V_h|_{\gamma_{ij}}, \quad i \neq j,\ i, j = 1, 2, \cdots, m,$$

such that, $u_i := u|_{\Omega_i} \in V_h|_{\Omega_i}$ $(i = 1, 2, \cdots, m)$ *satisfy the following splitting subproblem form:*

$$\begin{aligned} \alpha^h_{\Omega_i}(u_i,\ v) \ &+ \sum_{1 \leq j \neq i \leq m} \lambda_{ij} \int^*_{\gamma_{ij}} u_i\, v\, ds = (f,\ v)_{\Omega_i} \\ &+ \sum_{1 \leq j \neq i \leq m} \int^*_{\gamma_{ij}} g_{ij}\, v\, ds, \qquad \forall\ v \in V_h|_{\Omega_i}. \end{aligned} \tag{3.146}$$

Proof. Notice that $\{\varphi_b\}_{b \in \mathcal{N}_h}$ is the node basis of the finite element space V^h. Then, it is easy to see that the finite element problem (3.138) is equivalent to the following system (3.147):

$$\alpha^h_{\Omega}(u,\ \varphi_b) = (f,\ \varphi_b)_{\Omega}, \qquad \forall\ b \in \mathcal{N}_h. \tag{3.147}$$

Notice that $\varphi_b(x)$ only has a small support set, we then have from (3.147) that

$$\begin{aligned} \alpha^h_{\Omega_i}(u,\ \varphi_b) \ &= \ (f,\ \varphi_b)_{\Omega_i}, \quad \forall b \in (\mathcal{N}_h \cap \bar{\Omega}_i) \backslash \Sigma \\ \alpha^h_{\Omega_i}(u,\ \varphi_b) \ &- \ (f,\ \varphi_b)_{\Omega_i} = -\ [\alpha^h_{\Omega_i^c}(u,\ \varphi_b) - (f,\ \varphi_b)_{\Omega_i^c}], \\ &\qquad\qquad \forall\ b \in \mathcal{N}_h \cap \gamma_{ij},\ j \neq i \end{aligned} \tag{3.148}$$

where $\Omega_i^c = \Omega \backslash \bar{\Omega}_i$, i.e., the complement set of $\bar{\Omega}_i$ in Ω. We then define $g_{ij}^* \in V_h|_{\gamma_{ij}}$ $(j \neq i)$ satisfying that

$$G_{ij}^b = -\frac{\mathbf{n}}{s}[\alpha_{\Omega_i^c}(u, \varphi_b) - (f, \varphi_b)_{\Omega_i^c}]$$

$$g_{ij}^*(b) = \lambda_{ij}\, u(b) + G_{ij}^b, \qquad \forall b \in \mathcal{N}_h \cap \gamma_{ij}\ j \neq i$$

where $\mathbf{n}$ is the dimensional number of $\Omega \subset \mathcal{R}^n$ and s is the summation of $meas(e_f)$ for every face e_f of element, which is on the γ_{ij} and includes b as a nodal point (vertex). Thus, a direct computation implies that we have

$$\begin{aligned} \alpha_{\Omega_i}^h(u_i,\ \varphi_b) \ &+ \sum_{1\leq j\neq i\leq m} \lambda_{ij} \int_{\gamma_{ij}}^* u_i\, \varphi_b\, ds = (f,\ \varphi_b)_{\Omega_i} \\ &+ \sum_{1\leq j\neq i\leq m} \int_{\gamma_{ij}}^* g_{ij}^* \varphi_b\, ds, \quad \forall\, b \in \mathcal{N}_h \cap \gamma_{ij},\ j \neq i. \qquad (3.149) \end{aligned}$$

Hence, by the small support property of $\varphi_b(x)$, it is not hard to see that(3.146) can be obtained from (3.148) (3.149). This finishes the proof.

We now discuss the convergence of *Algorithm* . Let u be the solution of (3.138) and u_i^n $(1 \leq i \leq m)$ be the solutions of (3.143) at iterative step n, i.e., the *n-th* iterative approximations. Denote by

$$e^n \ := \ (u_i^n - u_i), \qquad u_i := u|_{\Omega_i} \qquad (3.150)$$

where e^n is the error at iterative step n. Therefore, by the *Algorithm* and Lemma

11, we obtain the error equations of the *Algorithm*: the errors $e_i^n \in V_h|_{\Omega_i}$, $i = 1, 2, \cdots, m$, satisfy

$$\alpha_{\Omega_i}^h(e_i^n,\ v) + \sum_{1\le j\ne i\le m} \lambda_{ij} \int_{\gamma_{ij}}^{*} e_i^n v ds = \sum_{1\le j\ne i\le m} \int_{\gamma_{ij}}^{*} \zeta_{ij}^n v\, ds, \quad \forall v \in V_h|_{\Omega_i} \quad (3.151)$$

$$\zeta_{ij}^{n+1}(b) = 2\lambda_{ij}\, e_j^n(b) - \zeta_{ji}^n(b), \quad \forall\, b \in \mathcal{N}_h \cap \gamma_{ij},\ 1 \le j \ne i \le m \qquad (3.152)$$

where

$$\zeta_{ij}^k = g_{ij}^k - g_{ij}^0, \qquad k = 1, 2, 3, \cdots. \qquad (3.153)$$

THEOREM 11 *Let* $u \in V_h$ *be the solution of the finite element linear system* (3.138). *Let* $u_i^n \in V_h|_{\Omega_i}$ $(i = 1, 2, \cdots, m)$ *be the solutions of (3.143) of the Algoritm at iterative step* n. *Then, for any initial* $g_{ij}^0 \in V_h|_{\gamma_{ij}}$ $(i \ne j,\ j = 1, 2, \cdots, m)$, *we have that*

$$\left(\sum_{i=1}^{m} ||u_i^n - u||_{H^1(\Omega_i)}^2\right)^{1/2} \longrightarrow 0, \qquad as\ \ n \to \infty.$$

Proof. First of all, we need to introduce a special norm for $\zeta = (\zeta_{ij})_{1\le i\ne j\le m}$ as follows.

$$|||\zeta||| = \sum_{1\le i\ne j\le m} \frac{1}{\lambda_{ij}} \int_{\gamma_{ij}} |\zeta_{ij}|^2\, ds, \qquad \zeta = (\zeta_{ij})_{1\le i\ne j\le m}$$

Taking $v = e_i^n \in V_i$ in (3.151), we have that,

$$\alpha_{\Omega_i}(e_i^n,\ e_i^n) = \sum_{1\le j\ne i\le m} \int_{\gamma_{ij}}^{*} (\zeta_{ij}^n - \lambda_{ij} e_i^n)\, e_i^n\, ds \qquad i = 1, 2, \cdots, m. \qquad (3.154)$$

Hence, from (3.152) and (3.154),

$$\begin{aligned}
|||\zeta^{n+1}|||^2 &= \sum_{i=1}^{m} \sum_{1\le j\ne i\le m} \frac{1}{\lambda_{ij}} \int_{\gamma_{ij}}^{*} |\zeta_{ij}^{n+1}|^2\, ds \\
&= \sum_{i=1}^{m} \sum_{1\le j\ne i\le m} \frac{1}{\lambda_{ij}} \int_{\gamma_{ij}}^{*} |2\lambda_{ij}\, e_j^n - \zeta_{ji}^n|^2\, ds \\
&= \sum_{i=1}^{m} \sum_{1\le j\ne i\le m} \frac{1}{\lambda_{ij}} \int_{\gamma_{ij}}^{*} |\zeta_{ji}^n|^2\, ds \\
&\quad - 4 \sum_{i=1}^{m} \sum_{1\le j\ne i\le m} \int_{\gamma_{ij}}^{*} (\zeta_{ji}^n - \lambda_{ji} e_j^n)\, e_j^n\, ds \\
&= \sum_{j=1}^{m} \sum_{1\le i\ne j\le m} \frac{1}{\lambda_{ji}} \int_{\gamma_{ji}}^{*} |\zeta_{ji}^n|^2\, ds \\
&\quad - 4 \sum_{j=1}^{m} \sum_{1\le i\ne j\le m} \int_{\gamma_{ij}}^{*} (\zeta_{ji}^n - \lambda_{ji} e_j^n)\, e_j^n\, ds \\
&= |||\zeta^n|||^2 - 4 \sum_{j=1}^{m} \alpha_{\Omega_j}^h(e_j^n, e_j^n),
\end{aligned}$$

where $\lambda_{ij} = \lambda_{ji} > 0$ and $\gamma_{ij} = \gamma_{ji}$ have been used. Then, we have that, for any positive integer M,

$$\sum_{j=0}^{M} \left(\sum_{i=1}^{m} \alpha_{\Omega_i}^h(e_i^n, e_i^n) \right) = \frac{1}{4} \left(|||g^0|||^2 - |||g^{M+1}|||^2 \right) \ge 0.$$

This clearly implies that

$$\sum_{i=1}^{m} \alpha_{\Omega_i}^{h}(e_i^n, e_i^n) \longrightarrow 0, \quad as \quad n \to \infty, \tag{3.155}$$

Hence, this together with (3.150) and (3.139) implies the theorem.

Furthermore, [24] has shown that, if taking

$$\lambda_{ij} = \lambda_{ji} = \lambda = O(h^{-1}), \qquad \forall\, 1 \le i \ne j \le m,$$

the contractor of the parallel iterative procedure algorithm for the nonconforming linear finite element approximations is $O(1 - C(\frac{h}{\tau})^{1/2})$. This means that the algorithm can have a contractor independent of h and τ if as usual choosing $\tau = O(h)$. We think that this result is still true for the conforming linear finite element approximations, which will be discussed in somewhere else later. Therefore, for higher dimension spatial domain cases, this method may be expected to be a good choice to solve the key linear systems in the numerical schemes defined in last sections.

Remarks 3.4.1: If we consider the model with both diffusion and advection, then the related elliptic partial differential problem has the following bilinear form in its weak formulation

$$\alpha_{\Omega}(v,\ w) - (\mathbf{q}\, v, w)_{\Omega}. \tag{3.156}$$

It is not difficult to check that the analyses and results of this section are still true if the bilinear form (3.156) is coercive. In fact, from **Remark 2.3.1**, **Remark 2.3.2**, **Remark 3.2.2.3**, **Remark 3.2.3.2** and **Remark 3.3.1**, the bilinear form (3.156) is coercive if either $\mathbf{q}$ is not large or μ is large enough or τ is small enough. We think this parallel procedure can also be extended to the situation for the *upwind* scheme discretization of the model with both diffusion and advection.

Chapter 4

Modeling a Fish Population in a Spatial Environment

This chapter is to model a fish population in a spatially heterogeneous environment by using the mathematical models and analyses developed in Chapter 2 and the numerical simulation techniques developed and analyzed in Chapter 3. Fish are assumed to live and move in a closed bounded environment where spatial variation occurs in the temporal-spatial variations of the usual environmental variables, temperature and dissolved oxygen concentration, and resource density. The development and discussion will focus on the spatial aspects of population dynamics.

4.1 Introduction

It is known from biology that, for the most part, environmental variables, such as organic chemical toxicant, resource density, temperature and dissolved oxygen, affect the physiological processes of individuals, such as the feeding rate, assimilation rate, maintenance, growth and reproduction or death, but not the population level directly. It is after the effects on the physiological processes at the individual level have been assessed, and the individuals combined to form a population, that a study of the dynamics of the population is viable. Moreover, higher ecological organizational levels such as populations and communities are generally data deficient, while the ecology of individuals is better documented. This is because most of biological and ecological data are obtained from short term observations and experiments on individuals. Therefore, in general, population and higher level models are best represented by employing an individual-based approach.

Individual-based, physiologically structured population models have been developed by several research groups (cf. [47, 50, 71, 72, 81, 83, 92, 95]). Their approach to model individual dynamics is based on energy budget techniques (cf. [71]). However, to the best of our knowledge, almost all the work, except Hallam *et al* [50] and [83], haven't considered the effects of spatial heterogeneity. Since the natural environment is usually spatially heterogeneous, the spatial component is very important for natural populations and communities, but, generally, difficult to analyze in models. In particular, it is more difficult to analyze spatial heterogeneity in the models which include diffusion. Hallam *et al* [50] and [83] have considered the spatial heterogeneity of the population models including only advective movement by using the method of characteristics. The discussions of Hallam *et al* [50] and [83] are based on the fact that the partial differential equations of the population models are quasi-linear hyperbolic while the spatial variable is just simply regarded as a dimension in physiologically-structured fish models. Unfortunately, this fact is no longer true for the population models including diffusive movements.

This chapter is to consider a fish population model with diffusion and advection in a spatially heterogeneous environment. For simplicity, spatial aspects of the model are mainly limited to spatial variability of the resource, and in the next chapter, chemical toxicant concentration as well. Fish are assumed to live and move in a closed bounded environment where variation occurs in the temporal-spatial variations of the usual environmental variables, temperature and dissolved oxygen concentration, and the resource density, etc. The effects of these variables occur through environmental and food chain pathways. The development and discussion will focus on the spatial aspects of population dynamics. The numerical simulation schemes we will use are defined and analyzed in Chapter 3.

We first give a summary of the individual growth model and population dynamic model below.

4.2 A Physiologically–Based Fish Individual Model

A model that is individually-based is essential to study effects at the population or higher level because most of environmental variables affect the physiological processors of individuals and subsequently impact the behavior of the population as a whole. The model that we use for the dynamic behavior of an individual female fish is originally introduced by Hallam *et al* [47, 54]. Moreover, in our computational model, we also employed the modification to include the effects of changes in temperature and dissolved oxygen concentration (cf. [2, 9, 20, 27, 87]). The model has been parameterized for rainbow trout, *Oncorhynchus mykiss*, however, because of the generality of the energetics approach, it can be used for other species of fish with some necessary modifications. The details of the individual fish model are found in Chapter 1 or the references. We now give a very brief description.

The model assumes that the only input to the lipid and structure compartments is obtained from the assimilated lipid and structure of the food; that is, no synthesis of lipid occurs from proteins and carbohydrates. This is not, in general, a valid hypothesis but because of the small amount of carbohydrates in the fish and its diet, lipogenesis may be ignored. The density of the resource is denoted by X (g/m^3) and we assume that $X = X_L + X_S$ where X_L and X_S are the lipid and structural portions of the resource. The amount of resource that can be converted to viable energy is based on the assimilation efficiencies of the lipid and structure, represented by A_{0L} (*nondim*) and A_{0S} (*nondim*) in the model. The mass of lipid, m_L (g), and the mass of structure, m_S (g), in an organism are assumed to have both labile and nonlabile portions. The nonlabile structure, m_{PS}, represents protein and carbohydrates bound in somatic tissues and is assumed to be nondecreasing with age; the nonlabile lipid, ϵm_{PS}, is the portion of the lipid associated with protein in cell membranes. The labile portion of lipid, $(m_L - \epsilon m_{PS})$, and the labile portion of structure, $(m_S - m_{PS})$, are utilized as energy sources to support the energy demands of the individual. Energetic demands, D, of the organism include maintenance, energy cost associated with ingested food, activity and reproduction. Reproduction, which occurs once a year in a special time interval, consists of the transferring of mass from the individual for egg production and the associated energetic cost. The losses of energy due to maintenance, SDA, and activity are assumed to occur on a continuous time scale and those due to reproduction occur on a discrete time scale. Hence, on intervals where there is no reproductive loss the dynamics of lipid and structural mass of an individual can be modeled with two coupled differential equations as follows

$$\frac{dm_L}{dta} = g_L(t, a, m_L, m_S, x, \cdots)$$

$$\frac{dm_S}{da} = g_S(t, a, m_L, m_S, x, \cdots) \tag{4.1}$$

where "$\cdots$" in $g_L(t, a, m_L, m_S, x, \cdots)$ and $g_S(t, a, m_L, m_S, x, \cdots)$ means that the right side terms g_L and g_S may be modified when the effects of some environmental variables, such as temperature and dissolved oxygen concentration, are considered. The detailed definitions of g_L and g_S can be obtained in Chapter 1 of this thesis.

As usual, we assume that the embryonic stage is 51 *days*, i.e., $J = 51$ in the numerical experiments, but it has to be modified while the effects of some environmental variables are considered. For details on the feeding representation as well as the equations used to model maintenance, activity, reproduction, and their modifications under the effects of some environmental variables, we refer to Chapter 1 and the references which have been cited. The model has been parameterized for rainbow trout, *Oncorhynchus mykiss* (cf. [5, 28, 32, 51, 53, 104, 109, 112, 113, 116]). The parameter values are also obtained from Table 1 and Table 2 in Appendix.

4.3 Fish Population Dynamics

A dynamic population model based on physiological and movement behavior of individuals is needed so that the environmental effects can be determined at the individual level directly and then the effects at the population level can be ascertained. The population dynamics can be described by partial differential equations of extended Mckendrick-von Foerster type. Let $\rho = \rho(t, a, m_L, m_S, x)$

$(numbers/d \cdot g^2 \cdot m^n)$, number per age, per mass of lipid, per mass of structure, per volume of spatial environment and at time t and location x, be the population density function. Since we assume that fish don't move in the embryonic and juvenile stage, then the fish dynamic population model is, in the embryonic stage, i.e., $a \in (0, J]$,

$$\begin{aligned}\frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial a} + \frac{\partial(\rho\, g_L)}{\partial m_L} + \frac{\partial(\rho\, g_S)}{\partial m_S} &= -\mu\rho \\ &\text{for } \forall\ t \in [0,T], a \in (0,J], x \in \Omega,\end{aligned} \tag{4.2}$$

and in the older life stage, i.e., $a \in (J, A]$,

$$\begin{aligned}\frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial a} + \frac{\partial(\rho\, g_L)}{\partial m_L} + \frac{\partial(\rho\, g_S)}{\partial m_S} - \nabla\cdot(k\,\nabla\rho - \mathbf{q}\rho) &= -\mu\rho \\ &\text{for } \forall\ t \in [0,T], a \in (J,A], x \in \Omega,\end{aligned} \tag{4.3}$$

where μ is the mortality function, k is the diffusive coefficient, $\mathbf{q}$ is the advection function, and $g_L = g_L(t, a, m_L, m_S, x)$ and $g_S = g_S(t, a, m_L, m_S, x)$ are the growth rates (g/d) of the lipid and structural components of an individual respectively, and are given in the individual model. Moreover, for simplicity, we assume that individuals live in a linear habitat, i.e., $\Omega \subset R$. For instance, a linear habitat might be approximated in a coastline or a river environment.

The mortality function μ is assumed to have the form (cf. [47])

$$\mu = \mu_a + \mu_w + \mu_y + \mu_d,$$

where μ_a represents the mortality in the population due to age, μ_w represents weight-dependent mortality, μ_y represents the mortality due to the younger of the year and μ_d represents a density dependent mortality. The specific forms of these mortalities are defined in Section 3.3 of Chapter 3.

We will consider two kinds of diffusion (cf. [29, 93, 96]). One is the purely random walk dispersal, for this case,

$$k = constant, \quad \text{usually take } \; k = 1. \tag{4.4}$$

The other is the random plus density-dependent dispersal, for this case,

$$k \;=\; 1 + \kappa_p \hat{P} \,,$$

where κ_p is a constant and $\hat{P}$ stands for all adult fish which have fed, that is,

$$\hat{P} = \int_J^{A_m} \rho \, da.$$

The function $\mathbf{q} = \mathbf{q}(m_L, m_S, x, P, \cdots)$ in (4.3) is the advection movement velocity (m/d) and describes how an individual of age a, lipid mass m_L and structure mass m_S at location x alters its advection movement in response to environmental heterogeneity and energetic constraints. We assume that individuals tend to move towards neighboring areas with higher food densities. The resource-directed advective movement velocity of an individual will depend on the size of the individual, the energy gained, and the gradient of the resource at the position where the individual is located. In numerical simulations, we implement the following advection movement behavior

$$\mathbf{q} = \begin{cases} 0, & \text{if} \quad E > D \\ \kappa v_s \dfrac{\partial r}{\partial x}, & \text{if} \quad E \leq D \end{cases} \tag{4.5}$$

where κ is a positive constant that measures the tendency of fish to pursue food and represents the distance covered by the foraging predator per unit change in the food resource density. $\dfrac{\partial r}{\partial x}$ is the slope of the resource distribution. v_s is an average swimming velocity (m/d) of an individual with length L_f (m) and is given by $v_s = 8.64 \cdot 10^4 s L_f$ where s denotes the body lengths per second of the predator while performing sustained cruising. Advection movement behavior (4.5) represents the case in which fish do not change location when the energy gained, E, while foraging around location x, exceeds the energy demands, D, even if there are local changes in the food resource density. $\mathbf{q}$ determines the spatial advection movement of individuals relative to their location. If there are no local changes of the food resource density, or if $E > D$, then fish do not change foraging location and the speed at which fish encounter food is determined only from physiological constraints. Therefore, an individual fish of length L_f foraging at location x encounters food resource at a rate given by $\max\{\mathbf{q}, v_s\}$.

Furthermore, if we modify k and $\mathbf{q}$ as in (1.20) and (1.21), then the fish population dynamics model can be rewritten in unified form by combining (4.2) and (4.3) together.

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial a} + \frac{\partial(\rho\, g_L)}{\partial m_L} + \frac{\partial(\rho\, g_S)}{\partial m_S} - \nabla \cdot (\tilde{k}\, \nabla\rho - \tilde{\mathbf{q}}\rho) = -\mu\rho \qquad \text{for } \forall\, t \in [0,T], a \in (0,A], x \in \Omega. \tag{4.6}$$

In addition to the balance law equation (4.6) , we adjoin the initial conditions

$$\begin{aligned} \rho = 0 \quad \text{or} \quad (\tilde{k}\, \nabla\rho - \tilde{\mathbf{q}}\rho)\cdot\nu &= 0 \qquad \text{on} \quad \partial\Omega \\ \rho(0, a, m_L, m_S, x) &= \rho_0(a, m_L, m_S, x) \\ \rho(t, 0, m_{L_0}, m_{S_0}, x) &= \int_0^{A_m}\int_0^{\infty}\int_0^{\infty} \beta\rho(t, a, m_L, m_S, x)\, da\, dm_L\, dm_S \end{aligned} \tag{4.7}$$

where the first formula of (4.7) gives the boundary condition, which asserts no flux of population across the boundary of the habitat or no fish on the boundary of the habitat; and the last equality of (4.7), i.e., the renewal equation, represents the birth process, where $\beta = \beta(t, a, m_{L_0}, m_{S_0}, m_L, m_S)$ represents the expected number of eggs with lipid content m_{L_0} and structure content m_{S_0} born to an individual of age a with lipid content m_L and structure content m_S at time t. The details about the birth processor and its modification under the effects of temperature and dissolved oxygen concentration are given in Chapter 1 and the references which are mentioned in Chapter 1. Furthermore, in order to construct the numerical scheme by using finite element methods (cf. [15, 107, 63]), we also need rewrite (4.6) (4.7) as the following weak formulation (cf. [75, 34]): find $\rho \in V$ satisfying

$$
\begin{aligned}
&\left(\frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial a} + \frac{\partial (\rho\, g_L)}{\partial m_L} + \frac{\partial (\rho\, g_S)}{\partial m_S},\ w\right) + \alpha(\tilde{k},\ \rho,\ w) + (\tilde{\mathrm{q}}\, \rho,\ w) \\
&\quad = -(\mu\, \rho,\ w), \qquad \text{for } \forall\, w \in V,\ t \in [0,T],\ a \in (0,A] \\
&\rho(0,a,m_L,m_S,x) \ = \ \rho_0(a,m_L,m_S,x) \\
&\rho(t,0,m_{L_0},m_{S_0},x) \ = \ \int_0^{A_m}\int_0^{\infty}\int_0^{\infty} \beta\rho(t,a,m_L,m_S,x)\, da\, dm_L\, dm_S
\end{aligned}
\tag{4.8}
$$

where $V = H_0^1(\Omega)$ or $V = H^1(\Omega)$ is defined same as previously, and $\alpha(\cdot,\cdot,\cdot)$ and $(\cdot,\cdot)$, etc. are also defined previously.

4.4 Numerical Computation Procedure

In this section, we develop a numerical computation procedure for the fish model defined in the last two sections. The numerical computation procedure is based on the basic ideas and analyses for the mathematical and computational models developed in Chapter 2 and Chapter 3. We utilize the implicit Runge-Kutta method for the ordinary differential system of fish individual model because of stiffness (cf. [76, 86]). For the partial differential problem of fish population dynamic model, we use a characteristic finite difference in the age-time domain and a finite element method with numerical integration and upwind modification for advection terms if necessary in the spatial domain (cf. [15, 63, 61, 64, 107]).

To construct the numerical computation procedure, we first partition the time domain (interval) $(0,T]$, age domain (interval) $[0,A_m]$ and the spatial domain $\Omega = (0,\ L)$ as follows.

$$\begin{aligned} 0 &= t_0 < t_1 < t_2 < \ldots < t_{N_t} = T \\ 0 &= a_0 < a_1 < a_2 < \ldots < a_{N_a} = A_m \\ 0 &= x_0 < x_1 < x_2 < \ldots < x_{N_h+1} = L \end{aligned} \tag{4.9}$$

where

$$\begin{aligned} t_i &= t_0 + i \cdot \tau = t_0 + i \cdot \frac{T - t_0}{N_t}, \quad i = 1, 2, \cdots, N_t \\ a_i &= a_0 + i \cdot \tau = a_0 + i \cdot \frac{A_m}{N_a}, \quad i = 1, 2, \cdots, N_a \\ x_i &= x_0 + i \cdot h = x_0 + i \cdot \frac{L}{N_h + 1}, \quad i = 1, 2, \cdots, N_h. \end{aligned} \tag{4.10}$$

Let $\mathcal{N}_h$ be the set of true finite element nodal points.and $V_h \subset V = H_0^1(\Omega)$ be the linear finite element approximate space and $\{\varphi_b\}_{b \in \mathcal{N}_h}$ be the standard finite element basis functions of V_h. Then, the numerical approximate scheme is defined as follows.

$$\begin{cases} m_L^j = m_L^{j-1} + g_L(a_j + \frac{1}{2}\tau, \frac{1}{2}(m_L^{j-1} + m_L^j), \frac{1}{2}(m_S^{j-1} + m_S^j), b) \\ m_S^j = m_S^{j-1} + g_L(a_j + \frac{1}{2}\tau, \frac{1}{2}(m_L^{j-1} + m_L^j), \frac{1}{2}(m_S^{j-1} + m_S^j), b) \end{cases}$$

$$\text{for} \quad \forall \ \ b \in \mathcal{N}_h, \ j = 1, 2, \cdots, N_a \tag{4.11}$$

$$m_L^0 = m_{L_0}(b), \qquad \text{for} \quad \forall \ \ b \in \mathcal{N}_h$$

$$m_S^0 = m_{S_0}(b), \qquad \text{for} \quad \forall \ \ b \in \mathcal{N}_h$$

And, for $1 \leq j \leq N_a$ and $1 \leq n \leq N_t$, seeking

$$\rho_h^{n,j} = \sum_{b \in \mathcal{N}_h} \rho_h^{n,j}(b)\varphi_b = \sum_i \rho_h^{n,j}(i)\varphi_i \in V_h \tag{4.12}$$

such that

$$\begin{aligned} \frac{\rho_h^{n,j}(b) - \rho_h^{n-1,j-1}(b)}{\tau} &= -\tilde{\mu}_h^{n-1,j}(b)\, \rho_h^{n,j}(b), \quad \forall\, b \in \mathcal{N}_h \\ & 1 \leq j \leq N_j,\ 1 \leq n \leq N_t \end{aligned} \tag{4.13}$$

$$\begin{gathered} (\tilde{\partial}_\tau \rho_h^{n,j},\ w)_h + \alpha_h(\tilde{k}_h^{n-1}, \rho_h^{n,j}, w) + (\tilde{\mathbf{q}}_h^{n,j}\ \rho_h^{n,j}, \nabla w)_h = -(\tilde{\mu}_h^{n-1,j} \rho_h^{n,j}, w)_h, \\ \forall\, w \in V_h,\ \ N_j < j \leq N_a,\ 1 \leq n \leq N_t \end{gathered} \tag{4.14}$$

$$\begin{aligned} &\rho_h^{0,j} = \pi_h \rho(a_j, m_{L_0}, m_{S_0}, x), \quad \forall\, 1 \leq j \leq N_a \\ &P_h^0 = \frac{1}{2}\rho_h^{0,0}\tau + \sum_{j=1}^{Na-1} \rho_h^{0,j}\tau \\ &\rho_h^{n,0} = \frac{1}{2}\tilde{\beta}_h^{n-1,0}\rho_h^{n,0}\tau + \sum_{j=1}^{N_a-1} \tilde{\beta}_h^{n-1,j}\rho_h^{n,j}\tau \\ &P_h^n = \frac{1}{2}\rho_h^{n,0}\tau + \sum_{j=1}^{N_a-1} \rho_h^{n,j}\tau, \quad \forall\, 1 \leq n \leq N_t \end{aligned} \tag{4.15}$$

where

$$\begin{aligned} \tilde{\mathbf{q}}_h^{n,j} &= \mathbf{q}(t_n, a_j, \cdots) \\ \tilde{\mu}_h^{n-1,j} &= \mu(t_n, a_j, \cdots, x, P^{n-1}) + \left.\frac{\partial g_L}{\partial m_L}\right|_{(t_n, a_j, \cdots, x)} + \left.\frac{\partial g_S}{\partial m_S}\right|_{(t_n, a_j, \cdots, x)} . \end{aligned}$$

Clearly, the third equation of (4.15) is a numerical simulation of the birth process.

Moreover, some parameters and functions should be modified as in Section 1.3 of Chapter 1 if the effects of temperature and dissolved oxygen concentration are considered (cf. [87]). Notice that the finite element partition is 1-*dimension* uniform, so the (4.14) can be rewritten for the explicit linear system, for the case of $\rho = 0$,

$$\begin{aligned}
&\frac{\rho_h^{n,j}(i) - \rho_h^{n-1,j-1}(i)}{\tau} - \left(\frac{\tilde{k}_h^{n-1}(i-1) + \tilde{k}_h^{n-1}(i)}{2h^2} + \frac{\tilde{\mathrm{q}}_h^{n,j}(i-1)}{2h} \right) \\
&\rho_h^{n,j}(i-1) + \left(\frac{\tilde{k}_h^{n-1}(i-1) + 2\tilde{k}_h^{n-1}(i) + \tilde{k}_h^{n-1}(i+1)}{2h^2} \right) \rho_h^{n,j}(i) \\
&- \left(\frac{\tilde{k}_h^{n-1}(i) + \tilde{k}_h^{n-1}(i+1)}{2h^2} - \frac{\tilde{\mathrm{q}}_h^{n,j}(i+1)}{2h} \right) \rho_h^{n,j}(i+1) \\
&= -\tilde{\mu}_h^{n-1,j}(i)\, \rho_h^{n,j}(i), \qquad \forall\, 1 \le i \le N_h,\ N_j < j \le N_a,\ 1 \le n \le N_t
\end{aligned} \tag{4.16}$$

where $f(i)$ represents $f(x_i)$, and

$$\begin{aligned}
\rho_h^{n,j}(0) &= 0, \quad \forall\, N_j < j \le N_a,\ 1 \le n \le N_t \\
\rho_h^{n,j}(N_h+1) &= 0, \quad \forall\, N_j < j \le N_a,\ 1 \le n \le N_t
\end{aligned}$$

For the case of Neumann boundary condition $(\tilde{k}\, \nabla\rho - \tilde{\mathrm{q}}\rho) \cdot \nu = 0$, except for (4.16), we have to add equations on the boundary, for $i = 0$,

$$\begin{aligned}
&\frac{\rho_h^{n,j}(0) - \rho_h^{n-1,j-1}(0)}{\tau} + \left(\frac{\tilde{k}_h^{n-1}(0) + \tilde{k}_h^{n-1}(1)}{h^2} + \frac{\tilde{\mathrm{q}}_h^{n,j}(0)}{h} \right) \rho_h^{n,j}(0) \\
&- \left(\frac{\tilde{k}_h^{n-1}(0) + \tilde{k}_h^{n-1}(1)}{h^2} - \frac{\tilde{\mathrm{q}}_h^{n,j}(0)}{h} \right) \rho_h^{n,j}(1) = -\tilde{\mu}_h^{n-1,j}(0)\, \rho_h^{n,j}(0)
\end{aligned}$$

and, for $i = N_h + 1$,

$$\begin{aligned}
&\frac{\rho_h^{n,j}(N_h+1) - \rho_h^{n-1,j-1}(N_h+1)}{\tau} - \left(\frac{\tilde{k}_h^{n-1}(N_h) + \tilde{k}_h^{n-1}(N_h+1)}{h^2} + \frac{\tilde{\mathbf{q}}_h^{n,j}(N_h)}{h}\right) \\
&\rho_h^{n,j}(N_h) + \left(\frac{\tilde{k}_h^{n-1}(N_h) + \tilde{k}_h^{n-1}(N_h+1)}{h^2} - \frac{\tilde{\mathbf{q}}_h^{n,j}(N_h+1)}{h}\right)\rho_h^{n,j}(N_h+1) \\
&= -\tilde{\mu}_h^{n-1,j}(N_h+1).
\end{aligned}$$

As we have mentioned in Chapter 3, we need to modify (4.16) by using the *upwind scheme* if there is advection to be considered. The corresponding *upwind* numerical scheme of (4.16) is defined as follows.

$$\begin{aligned}
&\frac{\rho_h^{n,j}(i) - \rho_h^{n-1,j-1}(i)}{\tau} + B_{i-1}^{n,j}\,\rho_h^{n,j}(i-1) + B_i^{n,j}\,\rho_h^{n,j}(i) \\
&-B_{i+1}^{n,j}\,\rho_h^{n,j}(i+1) = -\tilde{\mu}_h^{n-1,j}(i)\,\rho_h^{n,j}(i), \qquad (4.17) \\
&\qquad\qquad \forall\, 1 \le i \le N_h,\ N_j < j \le N_a,\ 1 \le n \le N_t
\end{aligned}$$

where $B_{i-1}^{n,j}$, $B_i^{n,j}$ *and* $B_{i+1}^{n,j}$ are obtained from the corresponding coefficients of (4.16) by *upwind* correction, which are defined explicitly in the following

$$\begin{aligned}
B_{i-1}^{n,j} &= -\frac{\tilde{k}_h^{n-1}(i-1) + \tilde{k}_h^{n-1}(i)}{2h^2} - \frac{1}{2h}\max(\tilde{\mathbf{q}}_h^{n,j}(i), 0) \\
B_i^{n,j} &= \frac{\tilde{k}_h^{n-1}(i-1) + 2\tilde{k}_h^{n-1}(i) + \tilde{k}_h^{n-1}(i+1)}{2h^2} \\
&\quad + \frac{1}{2h}\left(\max(\tilde{\mathbf{q}}_h^{n,j}(i), 0) - \min(\tilde{\mathbf{q}}_h^{n,j}(i), 0)\right) \\
B_{i+1}^{n,j} &= -\frac{\tilde{k}_h^{n-1}(i) + \tilde{k}_h^{n-1}(i+1)}{2h^2} + \frac{1}{2h}\min(\tilde{\mathbf{q}}_h^{n,j}(i), 0)
\end{aligned}$$

and the equations on the boundary end points do not need to be changed. The approximation and convergence of above numerical scheme have been analyzed in Chapter 3. Thus, the above numerical scheme (4.11)–(4.15) together with some modifications, for instance, the modifications due to the effects of temperature, consists of a computational model for a fish population with diffusion and advection in a spatially heterogeneous environment.

4.5 Numerical Experiments

The numerical simulations are conducted by solving the computational model developed in last section. The model has been parameterized for rainbow trout, *Oncorhynchus mykiss.* The habitat, $\Omega = (0, L)$, in which the populations live is taken to be 1 Km long and is divided into 10 equal length cells. The resource density is assumed to be homogeneous within the cells. These simulations were carried out with several cases of the resource distributions (homogeneous or heterogeneous step function distribution), movement types (different diffusion or diffusion-advection) and boundary conditions (Dirichlet or Neumann), etc. We mainly focus on investigating the dynamics of the fish population time-space distribution as they are viewed through the fish population density, total fish biomass, total fish age, total fish lipid, total fish structure (protein) and total fish protected protein.

We have not found any laboratory or field experimental data or computational simulation results for the above individual-based fish population models. Moreover, we have barely even found computational simulation samples for the age-structured fish population with diffusion and advection, although there are several numerical theoretical analysis studies for some special cases. Therefore, to test and apply our models, we design several typical cases from simple to complicated. For the simple cases, we may predict the reasonable computational results by applying biological, ecological and mathematical experiences. For the complicated case, we observe and analyze the computational results by comparing those of the simple cases as well as by applying biological, ecological and mathematical experiences. Furthermore, these experimental cases are also used to observe and analyze the chemical toxicant effects on fish population with diffusion and advection in the next chapter.

In the numerical simulations,we take the time-age step size $\tau = \frac{1}{20}$ *days* , the spatial mesh size $h = 0.0025Km$, and usually the simulation time $T \geq 5400$ *days*. For simplicity, we always assume that the initial population only occupies a small 1% interval at the middle of the habitat domain Ω.

Case 4.1. Consider the simple random walk dispersal diffusive movement (4.4), i.e. $k = 1$, and Dirichlet boundary condition $\rho = 0$ in a homogeneous no-toxicant spatially environment with resource level 5.00020×10^7 g/cm^3 (cf. Figure 8). We have observed the dynamics of the fish population temporal-spatial distribution because of the simple random walk dispersal diffusive movement. We have simulated 6000 *days*.

As we mentioned, we have chosen this case as a basic case, which will be used to compare the computational results of other cases. So, we have shown many figures to present the computational results (see Figure 9 – Figure 14). From these figures, the computational results seem to be reasonable in the viewpoints of mathematics, ecology and biology. The figures show that the behavior of population dynamics along the time-age characteristic direction in no-birth time period is similar as the behavior of the solution of a standard heat equation. After a long range time, about 3000 *days*, the distribution of fish population is almost uniform because of the homogeneity of the environment.

Case 4.2. This case is modified from *Case* 1 by using the Neumann boundary condition, $\tilde{k}\,\dfrac{\partial\rho}{\partial\nu} = 0$, to replace the Dirichlet boundary condition, $\rho = 0$.

The motivation to implement this case is to observe and compare the effects because of the boundary conditions. The results are presented in Figures 15 – 19. Comparing the results of these two cases, we have found they are similar in the middle of the domain. But, near the boundary, the case of Neumann boundary condition has more fish than those of Dirichlet case. This phenomenon matches our mathematical and biological expectations.

Case 4.3. This case is another modification of *Case* 1. We have used the random plus density-dependent dispersal, $k = 1 + \kappa_p \hat{P}$, to replace, the simple random dispersal, $k = 1$.

We have observed and compared the effects between the different diffusion types. The results are presented in Figures 20 – 23. The figures show that the behavior of fish population dynamics is very similar as that of case 4.1, except that fish spread in case 4.3 faster than that in case 4.1. This observation matches our mathematical, biological and ecological experiences and expectations.

Case 4.4. This is a case with heterogeneous environment, whose resource distribution is a step function (cf. Figure 8). Therefore, the model includes the diffusion as well as the possible advection movement induced by the food resource where the energy gained of fish is less than the energy demanded. We focus the advection movement effects on the dynamics of fish population because of the different resource level. The results are presented through Figures 24 – 26. The results show that in this case fish advection is not a continuous phenomenon, which matches our experiences and expectations of biology, since the fish density is not completely consistent with the resource density. This means that, the usual expectation of having the most fish where there is the most food resource, is not true in the whole time-space domain. By monitoring the computing, we have observed that fish make advection movement (4.5) mostly in the age period between 60 and 100 *days*. This matches the phenomenon in Figure 2 and 3 show that fish grow fastest in this age window.

4.6 Discussion and Future work

We have indicated a method to introduce individual variability due to environmental processes by coupling a heterogeneous spatial environment with the physiological processes of a fish population. We have studied the dynamics of the population with diffusion as well as with possible advection. We have compared two different movement behaviors, for example, different diffusion, different advection, etc.

Our method of this chapter can be extended to some dynamic resource cases, for instance, fish–*Daphnia* predator-prey model with immobile *Daphnia*. We hope we can do work in the parallel implementation of the model, test more cases, and observe physiological effects because of movements.

Chapter 5

Modeling Toxicant Effects on a Fish Population in a Spatially Heterogeneous Environment

This chapter models the chemical toxicant effects on a fish population in a spatially heterogeneous environment. Fish are assumed to live and move in a closed bounded environment where spatial variation occurs in the chemical toxicant concentration and in the resource density. The discussions of this chapter are based on the individual-based models developed in Chapter 4. We will consider both lethal and sublethal effects. The development and analysis will focus on the spatial aspects of population dynamics.

5.1 Introduction

Risk assessment is primarily developed for the higher organizational levels of ecological systems such as populations and communities (cf. [68, 94]). However, higher ecological organizational levels such as populations and communities are generally data deficient, while the toxicology and biology of individuals is better documented. This is because most of toxicological and biological data are derived from short term observations and experiments on individuals. Chemical impact occurs at the level of the individual, not at the population level, by affecting, directly or indirectly, individual processes such as the feeding rate, assimilation rate, maintenance, growth and reproduction or death of the individual. Even though the target site of a chemical may be specific tissues, the exposed, affected individual is the appropriate reference point for extrapolation to the population level. Hence, ecotoxicological models are best represented by using an individually–based approach, not an aggregated modeling technique.

Individual-based models have been effectively used to examine the effects of chemicals in aquatic organisms and populations (cf. [44, 48, 70, 72, 81, 83, 92, 95]), but the effects of spatial heterogeneity on chemically stressed systems almost have not been investigated except for Hallam *et al* [83]. However, since the natural environment is usually spatially heterogeneous, the spatial component is very important for natural populations, but, generally, very hard to analyze in models.

Moreover, it is more difficult to analyze spatial heterogeneity in the models which include diffusion. Hallam *et al* [83] has considered the spatial heterogeneity of the population models including only advective movement by using the method of characteristics. The discussions of [83] are based on the fact that the partial differential equations of the population models are quasi-linear hyperbolic while the spatial variable is just simply regarded as a dimension in a physiologically-structured fish models. Unfortunately, this fact is no longer true for population models including diffusion.

This chapter will model the chemical toxicant effects on a fish population in a spatially heterogeneous environment. The spatial aspects of the model are limited to spatial variability of the resource and toxicant concentration. Fish are assumed to live and move in a closed bounded environment where spatial variation occurs in the toxicant concentration and temporal-spatial variation in the resource density which is assumed to consist of identical individuals that do not move. Because of the mortality of the fish, the spatial variability in the toxicant, and the temporal-spatial variability in the resource, the toxicant exposure of an individual fish, which may occur through the environmental and food pathways, varies temporally.

The protocol used to study the effects of non-polar narcotic toxicant on a fish population, which is exposed to a spatially varying toxicant and has a dynamic resource, when toxic exposure occurs through the environmental and/or the food pathways, utilizes the following components:

- individual model
- toxicant exposure–effect model
- population model coupling temporal–spatial processes with physiological processes of individuals and a dynamic resource.

The basic form of the first and third model have been discussed in Chapter 4, we here only need do some small modifications to them. The basic ideas employed to assess chemical exposure and effects on individuals are discussed in [81]. A summary of these models is presented below to set the stage for this study on the effects of chemicals on populations living in spatially heterogeneous environments.

5.2 Exposure–Effect Model

The uptake of chemical from the environment and food represents the chemical exchange between the aqueous environment and the individual fish across the gill membranes and the chemical exchange between the fish and its intestinal food across the intestinal wall. The uptake model we use is a modification of FGETS, a model developed by Barber et al [4] to handle exposure of fish to non-polar, hydrophobic, reversible chemicals. The model was formulated based on the assumption that both environmental and food exposure are gradient-driven processes.

The mathematical model that describes the processes of chemical uptake from the environment and food and includes dilution of chemical due to organism growth is

$$\frac{dC_T}{da} = k_1 C_w + \frac{F}{W_T} C_F - k_2 C_T - \frac{E k_E}{W_T} C_A - \frac{1}{V}\frac{dV}{da} C_T \tag{5.1}$$

where C_T, C_w, C_F, and C_A are respectively the concentrations of chemical in the whole fish, in the environment, in the food, and in the aqueous portion of the organism. F is the weight of the food eaten per day and E is the weight of material defecated per day. k_E is the partition coefficient of chemical to excrement and is given by $k_E = \frac{C_E}{C_A}$, where C_E is the concentration of the chemical in the feces. k_1 and k_2 are the uptake and depuration rates of the environmental chemical, respectively, and are specified by

$$k_1 = S_g k_w V^{-1}, \;\; k_2 = S_g k_w V^{-1}(P_A + P_L K_L + P_S K_S)^{-1}.$$

k_w measures the conductivity of the exposed surface area, S_g, and V is the volume of the organism calculated by using the total weight, W_T, and the density of the organism. P_A, P_L and P_S are the aqueous, lipid, and structural fractions of the organism, respectively; K_L is the partition coefficient of the chemical between the organic lipid and water; K_S is the partition coefficient of the chemical between the organic structure and water. The last term in (5.1) represents the dilution of chemical due to organism growth. The parameters used in the uptake model can be found in Table 1, Table 2 and Table 3 in Appendix.

Hypotheses imposed in the model development include the following. An individual organism is assumed to be comprised of three chemical phases: aqueous, structural, and lipid. The structural component is generally viewed as being composed of (physiologically active) protein and carbohydrates. A second hypothesis is that the time scales for the exchange across the exposed surface area, S_g, are regarded as being much slower than the distribution of chemical within the organism. Using this assumption, C_A is expressed in terms of C_T via

$$C_T = (P_A + P_L K_L + P_S K_S) C_A.$$

A third hypothesis was imposed to deal with difficulties of the transient events during digestive processes. The simplest assumption that avoids most of these difficulties is that of equilibration of chemical between the organism's body and the gut contents. This assumption, however, is not necessarily true. Hallam et al. [46] have indicated that this is the worst case assumption during increasing body concentration when exposed to contaminated food (i.e., no more chemical could be taken up under any thermodynamically consistent assumption than would be taken up when food and body equilibrate). During depuration, however, this assumption leads to predicted minimum depuration times; that is, any other thermodynamically consistent assumption would lead to longer predicted depuration times. For toxicity evaluations, this would usually not be considered the worst case scenario.

To calculate the concentration of the chemical in the food, we assume instantaneous chemical equilibration with the water and within the organism. The food, like the consumer, consists of the aqueous, lipid and structural phases and the chemical is distributed among them according to its affinity for these phases.

Lethal Effects: To model the effects of chemicals on individuals we need to couple the uptake model with models for the mode of action and models for concentration–response relations. Effects of chemicals on individuals focus on mortality but sublethal effects, such as reduction of growth rate, could be considered using a similar method (cf. [43, 58, 67]). The assessment of mortality due to chemical action is implemented by utilizing formulations based upon quantitative structure–activity relations (QSARs). There are numerous QSARs in the literature for chemicals with different modes of action. We utilize results of Veith et al. [111] and Konemann [69] developed for baseline narcotic chemicals and relate a chemical property, the octanol/water partition coefficient, K_{ow}, to mortality of individuals (see Figure 1). For a single individual, an effect occurs when concentration of chemical in the aqueous phase reaches a critical level, denoted by LC_{50}, and is calculated from the equation $\log LC_{50} = -0.8 - \log K_{ow}$.

The exposure–effect model is coupled with the physiologically–based individual model which yields expressions for the weight and surface area of the organism.

This model of an individual fish includes lipid and structural components necessary for assessing effects of lipophilic chemicals on individuals. The aqueous component of an individual needed for the exposure model is assumed to be proportional to the structural mass of the individual.

Sublethal Effects: The chemical toxicant sublethal effects for fish have been discussed in [26], in which the same mechanism for the *Daphnia* is applied (cf. [48, 43, 67]). While the toxicant effect is sublethal, a reduction in the accumulation and growth due to sublethal chemical effects, say χ, need to be introduced to modify the individual fish model. We choose the reduced rate of accumulation of lipid and the reduced rate of growth of structure for individual fish are the same as ones for an individual *Daphnia* as follows.

$$\chi = \begin{cases} 1 & \text{if } C_A < 10^{-1.83} K_{ow}^{-1}, \\ 1 - \dfrac{1.37(C_A - 10^{-1.83} K_{ow}^{-1})}{0.0395 K_{ow}^{-1} + C_A} & \text{if } 10^{-1.83} K_{ow}^{-1} \le C_A \le 10^{-0.8} K_{ow}^{-1}, \\ 0 & \text{if } C_A > 10^{-0.8} K_{ow}^{-1}. \end{cases} \tag{5.2}$$

The value $10^{-1.83} K_{ow}^{-1}$ is the experimental no effect threshold. There is no effect on the growth of a fish, until C_A exceeds the threshold value $10^{-0.8} K_{ow}^{-1}$, the no growth threshold. While C_A exceeds this threshold, individual fish have a negative net growth rate, which only includes the loss functions.

Combined Effects: In our numerical simulations of Chapter 5, we consider the chemical toxicant effects combining the lethal and sublethal effects together. That is, the representation of chemical toxicant sublethal effects results in the growth reduction occurring continuously as a response to continuous internal toxicant concentration. Death of the organism caused by lethal toxicant effects is assumed to befall exactly at the time when the concentration in the aqueous phase of the fish reaches the value LC_{50} and, different from the growth, is quantally rather than continuously, assessed.

Finally, for simplicity in numerical treatment, we need rewrite the uptake equation as the following form.

$$\frac{dB_T}{da} = sk_w C_w + C_F F - \frac{B_T}{W_T\, BCF}(sk_w + Ek_E) \tag{5.3}$$

where $B_T = C_T \cdot W_T$ represents the total toxicant in the organism.

5.3 Individual-Based Population Model and Its Numerical Scheme

A dynamic population model based on physiological and movement behavioral aspects of individuals is needed so that the effects of chemical toxicants at the individual level can be determined directly and then the cumulative effect at the population level can be ascertained. The individual model must allow for relevant interactions between the individual and the chemical and must also be able to account for toxicity. Appropriate model components must be chosen with specific chemical and type of exposure in mind. For example, for lipophilic chemicals, the principal component of effect determination is the individual compartment of high affinity, the lipid compartment. The lipid in an individual acts as a buffer for lipophilic toxicants, allowing larger body burdens in fatter individuals than in less fat organisms. Lipid storage provides protection against stress from an acute exposure only if the organism does not mobilize stored lipid rapidly, such as during reproduction. Hence, to discuss the effects of toxicants, it is necessary to model the lipid content of an exposured organism. In addition to the lipid component, the individual model must consider a structure component to account for size related measurements such as weight or length of the organism. Structure is regarded as consisting primarily of protein and carbohydrates. Therefore, we need to modify the inidividual-based population model.

First, we need to modify the individual fish model defined in last Chapter 4 by adding the growth reduction rate χ as follows.

$$\begin{aligned} \frac{dm_L}{da} &= g_L \equiv \chi G_L - F_L \\ \frac{dm_S}{da} &= g_S \equiv \chi G_S - F_S \end{aligned} \tag{5.4}$$

where χ is defined in (5.2) for the sublethal effects and combined effects. However, for the lethal effects, fish die when the C_A reaches the value LC_{50}. The dynamic population model based on physiological and movement behavioral aspects of individuals has the same form as in Chapter 4.

$$\begin{aligned} \frac{\partial\rho}{\partial t} + \frac{\partial\rho}{\partial a} + \frac{\partial(\rho\, g_L)}{\partial m_L} + \frac{\partial(\rho\, g_S)}{\partial m_S} &= -\mu\rho \\ &\text{for } \forall\ t \in [0,T], a \in (0,J], x \in \Omega, \end{aligned} \tag{5.5}$$

$$\begin{aligned} \frac{\partial\rho}{\partial t} + \frac{\partial\rho}{\partial a} + \frac{\partial(\rho\, g_L)}{\partial m_L} + \frac{\partial(\rho\, g_S)}{\partial m_S} - \nabla\cdot(k\,\nabla\rho - \mathbf{q}\rho) &= -\mu\rho \\ \text{for } \forall\ t \in [0,T], a \in (J,A], x \in \Omega,& \end{aligned} \tag{5.6}$$

$$\begin{aligned} \rho = 0 \quad \text{or} \quad (\tilde{k}\,\nabla\rho + \tilde{\mathbf{q}}\rho)\cdot\nu &= 0 \qquad \text{on} \quad \partial\Omega \\ \rho(0,a,m_L,m_S,x) &= \rho_0(a,m_L,m_S,x) \\ \rho(t,0,m_{L_0},m_{S_0},x) &= \int_0^{A_m}\int_0^{\infty}\int_0^{\infty}\beta\rho(t,a,m_L,m_S,x)\,da\,dm_L\,dm_S \end{aligned} \tag{5.7}$$

where the function $\mathbf{q}$ will be defined later, and the others are same as in Chapter 4. For simplicity, we only consider the Dirichlet condition in our numerical experiments. The related parameters and functions in (5.4) – (5.7) may be modified due to the effects of temperature and dissolved oxygen.

Movement behavior of individuals can be very complicated. For simplicity, we here only consider the purely random walk dispersal (4.4) (cf. [29, 93, 96]). However, the advective movement is more complicated than that in Chapter 4 since individuals may alter their movement in response to changes in not only resource density but the concentration of contaminated media as well. In addition, exposured organisms may avoid contaminated media, may be attracted to contaminated media (e.g. pesticide–debilitated prey) or may lose their ability to detect contamination due to toxicant effects (cf. [82, 83, 105]). If the contamination is local and of short duration, avoidance can prevent the occurrence of effects on mobile organisms. However, avoidance of chronically contaminated media or food may result in lack of resource which can seriously affect the population. There is no standardized procedure for determining avoidance and preference behaviors largely because they depend on the chemical and its concentration as well as the species (cf. [39, 52]). Thus, we may asume that

$$\mathbf{q} = \mathbf{q}_r + \mathbf{q}_c \tag{5.8}$$

where $\mathbf{q}_r$ represents the advective movement velocity due to changes in food resource density and $\mathbf{q}_c$ represents the advection movement velocity due to changes in concentration of contaminated media. In the simulations, the function $\mathbf{q}_r$ is determined same as in Chapter 4, that is,

$$\mathbf{q}_r = \begin{cases} 0, & \text{if } \ E > D \\ \kappa v_s \dfrac{\partial r}{\partial x}, & \text{if } \ E \leq D \end{cases} \tag{5.9}$$

where κ is a positive constant that measures the tendency of fish to pursue food and represents the distance covered by the foraging predator per unit change in the food resource density. $\frac{\partial r}{\partial x}$ is the slope of the resource distribution. v_s is an average swimming velocity (m/d) of an individual with length $L_f\,(m)$ and is given by $v_s = 8.64 \cdot 10^4 s L_f$ where s denotes the body lengths per second of the predator while performing sustained cruising. Similarly, we assume that the function $\mathbf{q_c}$ can be defined as follows.

$$\mathbf{q_c} = \pm\, \kappa_0 v_s \frac{\partial C_w}{\partial x}, \tag{5.10}$$

where κ_0 is a positive constant that measures the tendency of fish to pursue food (prey) and represents the distance covered by the foraging fish per unit change in the concentration of contaminated media. C_w represents the concentration of contaminated media and $\frac{\partial C_w}{\partial x}$ denotes the derivative of C_w with respect to the variable x and represents the rate of change of the concentration of contaminated media at x. In (5.10), "+ "means that fish is attracted to contaminated media and "− "means that fish want to avoid the toxicants. If fish do not have the ability to detect contaminated media, then we assume that $\mathbf{q_c} = 0$. This advective movement induced by chemical toxicant has similar dynamic behavior as where winds blow a fume away.

The toxicant-population model is formulated so that a toxicant may be released at different locations with different levels and at numerous times for arbitrary exposure length, as a result we may obtain a spatially explicit variation in toxicant concentration. We ignore movement and transformation of toxicants in the environment and concentrate on the effects of stress on biota. The numerical procedure follows cohorts of individuals that move continuously in the heterogeneous habitat (heterogeneity results from both resource and toxicant distributions). This numerical procedure allows effects of spatially explicit toxicant exposure to be assessed at the individual level, but the overall effects can still be determined by an accumulation of individual effects.

We will develop a numerical computation scheme by modifying and extending (4.11) – (4.15) of Chapter 4. By using same notations, we can write the numerical computation scheme in the following.

$$\begin{cases} m_L^j &= m_L^{j-1} + g_L^j(a_j + \frac{1}{2}\tau, \frac{1}{2}(m_L^{j-1} + m_L^j), \frac{1}{2}(m_S^{j-1} + m_S^j), b) \\ m_S^j &= m_L^{j-1} + g_L^j(a_j + \frac{1}{2}\tau, \frac{1}{2}(m_L^{j-1} + m_L^j), \frac{1}{2}(m_S^{j-1} + m_S^j), b) \end{cases}$$

$$\text{for} \quad \forall \ b \in \mathcal{N}_h, \ \ j = 1, 2, \cdots, N_a \tag{5.11}$$

$$m_L^0 = m_{L_0}(b), \quad (given) \quad \text{for} \quad \forall \ b \in \mathcal{N}_h$$

$$m_S^0 = m_{S_0}(b), \quad (given) \quad \text{for} \quad \forall \ b \in \mathcal{N}_h$$

$$B_T^j = B_T^{j-1} + g_c(a_j + \frac{1}{2}\tau, \frac{1}{2}(B_T^{j-1} + B_T^j)),$$

$$\text{for} \quad \forall \ b \in \mathcal{N}_h, i = 1, 2, \cdots, N_a \tag{5.12}$$

$$B_T^0 = B_{T_0}(b), \quad (given) \quad \text{for} \quad \forall \ b \in \mathcal{N}_h$$

And, for $1 \leq j \leq N_a$ and $1 \leq n \leq N_t$, seeking

$$\rho_h^{n,j} = \sum_{b \in \mathcal{N}_h} \rho_h^{n,j}(b)\varphi_b = \sum_i \rho_h^{n,j}(i)\varphi_i \in V_h \tag{5.13}$$

such that

$$\begin{aligned} \frac{\rho_h^{n,j}(b) - \rho_h^{n-1,j-1}(b)}{\tau} &= -\tilde{\mu}_h^{n-1,j}(b)\, \rho_h^{n,j}(b), \quad \forall\, b \in \mathcal{N}_h \\ & \qquad 1 \leq j \leq N_j,\ 1 \leq n \leq N_t \end{aligned} \tag{5.14}$$

$$\begin{aligned} &(\tilde{\partial}_\tau \rho_h^{n,j},\, w)_h + \alpha_h(\tilde{k}_h^{n-1}, \rho_h^{n,j}, w) + (\tilde{\mathbf{q}}_h^{n,j}\, \rho_h^{n,j}, \nabla w)_h \\ &\quad = -(\tilde{\mu}_h^{n-1,j} \rho_h^{n,j}, w)_h, \forall\, w \in V_h, \quad N_j < j \leq N_a,\ 1 \leq n \leq N_t \end{aligned} \tag{5.15}$$

$$\begin{aligned} &\rho_h^{0,j} = \pi_h \rho(a_j, m_{L_0}, m_{S_0}, x), \quad \forall\, 1 \leq j \leq N_a \\ &P_h^0 = \frac{1}{2}\rho_h^{0,0}\tau + \sum_{j=1}^{Na-1} \rho_h^{0,j}\tau \\ &\rho_h^{n,0} = \frac{1}{2}\tilde{\beta}_h^{n-1,0}\rho_h^{n,0}\tau + \sum_{j=1}^{N_a-1} \tilde{\beta}_h^{n-1,j}\rho_h^{n,j}\tau \\ &P_h^n = \frac{1}{2}\rho_h^{n,0}\tau + \sum_{j=1}^{N_a-1} \rho_h^{n,j}\tau, \quad \forall\, 1 \leq n \leq N_t \end{aligned} \tag{5.16}$$

where

$$\begin{aligned} g_c &= S_g k_w C_w + C_F F - \frac{B_T}{W_T\, BCF}(S_g k_w + E k_E) \\ g_L^j &= (\tilde{\chi}^{j-1} G_L - F_L)\big|_{(a_j + \frac{1}{2}\tau, \frac{1}{2}(m_L^{j-1} + m_L^j), \frac{1}{2}(m_L^{j-1} + m_L^j), b)} \\ g_S^j &= (\tilde{\chi}^{j-1} G_S - F_S)\big|_{(a_j + \frac{1}{2}\tau, \frac{1}{2}(m_L^{j-1} + m_L^j), \frac{1}{2}(m_L^{j-1} + m_L^j), b)} \\ \tilde{\chi}^{j-1} &= \chi(B_T^{j-1}). \end{aligned}$$

Moreover, we need to modify (5.15) by the upwind technique because of the advection.

$$
\begin{aligned}
&\frac{\rho_h^{n,j}(i) - \rho_h^{n-1,j-1}(i)}{\tau} + B_{i-1}^{n,j}\, \rho_h^{n,j}(i-1) + B_i^{n,j}\, \rho_h^{n,j}(i) \\
&\qquad -B_{i+1}^{n,j}\, \rho_h^{n,j}(i+1) = -\tilde{\mu}_h^{n-1,j}(i)\, \rho_h^{n,j}(i), \qquad (5.17) \\
&\qquad \forall\, w \in V_h, \quad N_j < j \leq N_a, \ 1 \leq n \leq N_t
\end{aligned}
$$

where $B_{i-1}^{n,j}$, $B_i^{n,j}$ *and* $B_{i+1}^{n,j}$ are obtained from the corresponding coefficients of (4.16) by *upwind scheme* correction, which are defined explicitly in the following

$$
\begin{aligned}
B_{i-1}^{n,j} &= -\frac{\tilde{k}_h^{n-1}(i-1) + \tilde{k}_h^{n-1}(i)}{2h^2} - \frac{1}{2h} \max(\tilde{\mathrm{q}}_h^{n,j}(i), 0) \\
B_i^{n,j} &= \frac{\tilde{k}_h^{n-1}(i-1) + 2\tilde{k}_h^{n-1}(i) + \tilde{k}_h^{n-1}(i+1)}{2h^2} \\
&\quad + \frac{1}{2h}\left(\max(\tilde{\mathrm{q}}_h^{n,j}(i), 0) - \min(\tilde{\mathrm{q}}_h^{n,j}(i), 0)\right) \\
B_{i+1}^{n,j} &= -\frac{\tilde{k}_h^{n-1}(i) + \tilde{k}_h^{n-1}(i+1)}{2h^2} + \frac{1}{2h} \min(\tilde{\mathrm{q}}_h^{n,j}(i), 0)
\end{aligned}
$$

where $f(i)$ represents $f(x_i)$, and

$$
\begin{aligned}
\rho_h^{n,j}(0) &= 0, \quad \forall\, N_j < j \leq N_a, \ 1 \leq n \leq N_t \\
\rho_h^{n,j}(N_h + 1) &= 0, \quad \forall\, N_j < j \leq N_a, \ 1 \leq n \leq N_t
\end{aligned}
$$

Our numerical simulations are based on the above *upwind scheme.*

5.4 Effects of Toxicant on Population

The population model is investigated numerically with the nominal, unstressed simulations compared to the simulations with toxicant stress to indicate effects. Lassiter and Hallam [81] developed an approach to evaluate the effects of the lipid distribution in a population on population dynamics in response to an acute exposure of a lipophilic narcotic chemical. According to this theory, in an assessment of mortality, an individual with smaller lipid fraction content will die before another individual with a larger lipid fraction, given equal exposure. The theory of the survival of the fattest considers homogeneous toxic exposures to a static population that are necessarily acute. This theory is not valid when these assumptions are violated. In a dynamic setting, survival of the population after chronic exposure is determined not only by the lipid distribution, but also by the growth rate of the individuals in the population (cf. [48]).

In addition to physiological aspects of the population, the response of a fish population to a toxicant exposure depends on the spatial pattern of the toxicant and resource as related to the distribution of individuals in time and space, the duration of the exposure, as well as the strength of the toxicant. In many cases, the rate and the spatial–temporal pattern of release of chemicals from a source is the major source of uncertainty in an ecological risk assessment (cf. [82, 68, 94]). We consider inhomogeneous spatial distribution of the chemical toxicant, in fact, a step function distribution. We discuss several simple scenarios of heterogeneous chemical toxicant environment. As in Chapter 4, we assume the habitat in which the populations live is taken to be 1 Km long and is equally divided into 10 cells. We incorporate release of the chemical in our model by dividing the habitat into cells that are assumed environmentally homogeneous. For the following simulations, since we do not have any any laboratory or field experimental data or computational simulation results for the model, we will compare the computational results to those for the population model obtained by Chapter 4. We mainly focus on the spatial–temporal distribution of fish population as they are viewed through the fish population density, total fish biomass, total fish age, total fish lipid, total fish structure (protein) and total fish protection protein. In particular, the dynamics of population variations are due to the advection induced by the toxicant. We consider the combined effects of lethal effects and sublethal effects. In the numerical simulations, we take the time-age step size $\tau = \frac{1}{20}\ days$, the spatial mesh size $h = 0.0025\ Km$, the simulation time $T \geq 5400\ days$. For simplicity, we always assume that the initial population only occupies a small 1% interval at the middle of the habitat domain Ω.

To demonstrate the effects of chemicals and the importance of chemical heterogeneity, we stress the theoretical population employing the same chemical, and we investigate the outcomes by varying the spatial distribution of the environmental chemical concentration and the initial time of exposure. The structure of the population is compared before and after the exposure and the time evolution of the stressed population is compared to the nominal, unstressed population. In our numerical experiments, we design the following four cases to implement the models developed in Chapter 2 and Chapter 3. We have considered the combined effects of lethal toxicant effects and sublethal toxicant effects. For the toxicant induced movements, we have discussed the the scenarios that fish is attracted to the contaminated media (chemical toxicant), that is, $\mathbf{q}_c > 0$, and fish try to avoid the contaminated media (chemical toxicant), that is, $\mathbf{q}_c < 0$. We consider the simple random walk dispersal diffusion (4.4), i.e. $k = 1$, and Dirichlet boundary condition $\rho = 0$. As in Chapter 4 for the population model, we always assume the initial population only occupies a small 1% interval at the middle of the habitat domain Ω. We assume the chemical with $K_{ow} = 10^5$ and combined effects.

Case 5.1. Consider the heterogeneous environment with a step function chemical toxicant distribution (see Figure 27) but uniform resource level 5.00020×10^{-7} g/cm^3 (see Figure 8). The chemical exposure begins at 1400 *days* and is never turned off. Fish try to avoid the chemical, that is, the advection term $\mathbf{q}_c < 0$. The computational results are shown in Figures 28 – 30. The figures show that the chemical induced advection, which dominates the diffusion, is a continuous movement like winds blowing a fume. The population persists to 5400 *days*, so the population could recover if the chemical is turned off.

Case 5.2. This case has the same environment as *case 5.1.* But, the chemical toxicant advection is opposite, the advection term $\mathbf{q}_c > 0$, that is, fish are attracted by the chemicals. The chemical exposure begins at 1400 *days* and is never turn off. The computational results are shown in Figure 31 – Figure 33. Like *Case 5.1*, the figures show that the chemical induced advection, which dominates the diffusion, is a continuous movement.The population goes to extinction at 3500 *days*.

Case 5.3. Consider the heterogeneous environment with a step function chemical toxicant distribution (see Figure 8) and a step function resource distribution (see Figure 27). We consider both resource induced advection and chemical induced advection. Fish try to avoid the chemicals. The chemical exposure begins at 1400 *days* and is never turned off. The computational results are shown in Figures 34 – 36. The figures show that the chemical induced advection, which is a continuous movement, dominates both the diffusion and resource induced advection. The population persists to 5400 *days*. So, the population could recover if the chemical is turn off. However, we have also tested the situation by the other heterogeneous resource distribution (see Figure 8) to replace resource distribution (see Figure 27). The fish population goes to extinction at 4000 *days* because the resource level is too low under the low toxicant level.

Case 5.4. This case is also the heterogeneous environment with a step function chemical toxicant distribution and a step function resource distribution (see Figure 27). But, in this case, fish are attracted by the chemicals. The chemical exposure begins at 1400 *days* and is never turned off. The computational results are shown in Figures 37 – 39. The figures show that the advection is a dominated continue movement. The population persists to 5400 *days*, so the population could recover if the chemical is turned off. This case simulates the situation where the food resource contained a chemical appealing to fish.

5.5 Discussion and Further Work

We have indicated a method to study the effects of non-polar narcotic chemicals on a fish population exposed to a spatially varying chemical and a possible varying resource. We have demonstrated in the assessment of mortality that the spatial pattern of the toxicant and resource, as related to the distribution of individuals in time and space, can influence the physiological structure of the population and determine the survival or extinction of the population. An implication of the current study is that, in addition to the biological attributes of the population, spatial heterogeneity is essential to determine the effects of a toxicant on the population.

Our method of this chapter can be extended to some dynamic resource cases, for instance, fish–*Daphnia* predator-prey model with immobile *Daphnia*, in which the toxicant effects are very complicated (cf. [26]), since the toxicant effects may occur on one or both of them. We hope we can do work in the parallel implementation of the model, test more cases, and observe physiological effects because of movements.

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Appendix

Table 1: Parameter values and units in the individual model (I)

Symbol	*Interpretation*	*Value (unit)*	*Source*
A_{0L}	lipid assimilation efficiency	0.85 (nondim)	[5, 31, 32, 104]
A_{0S}	structure assimilation efficiency	0.684 (nondim)	”
A_3	labile lipid mobilization rate	0.013 (d^{-1})	[109]
A_4	labile structure mobilization rate	0.028 (d^{-1})	”
ϵ	fraction lipid associated with nonlabile structure	0.12 (nondim)	[104]
M_p	mass of prey	2.7×10^{-4} (g)	[70]
L_p	length of prey	$0.34 \times 10-2$ (m)	”
β	as in $m_{ps} = \beta m_s$	0.71 (nondim)	[104]
β_2	proportionality constant for wetted surface area	0.4 (nondim)	[116]
q	swimming efficiency	0.2 (nondim)	[33]
a	as in $s_d = [aL_p + b]L_f^{\frac{1}{2}}$ for reaction distance	75 ($m^{-\frac{1}{2}}$)	[8]; [112, 113]
b	as in $s_d = [aL_p + b]L_f^{\frac{1}{2}}$ for reaction distance	0.52 ($m^{\frac{1}{2}}$)	”
β_1	isometric constant relating weight to length	17×10^2 ($g\,m^{-3}$)	[28, 104, 116]

Table 2: Parameter values and units in the individual model (II)

Symbol	*Interpretation*	*Value (unit)*	*Source*
s_p	burst swimming velocity	4.0 ($length/sec$)	[6]
k_0	as in $k = k_0 m_{ps}^{k_1}$	16.5 ($g^{0.7} \cdot d^{-1}$)	[40, 104]
k_1	as in $k = k_0 m_{ps}^{k_1}$	0.7 (nondim)	[40]
d_p	as in $M_g = d_p V_g$ density of prey (dry wt)	0.052 ($g \cdot cm^{-3}$)	[50, 82]
c	as in $V_g = c\, m_{ps}$ for gut volume	0.864 ($cm^3\, g^{-1}$)	[40, 104]
e_m	minimum lipid per egg	3.2×10^{-3} (g)	[53, 102]
e_M	maximum lipid per egg	1.02×10^{-2} (g)	"
e_s	structure per egg	2.38×10^{-2} (g)	[51, 102]
σ	slope of egg equation	67.2×10^{2} (m^{-1})	[12]
η	minimum length for reproduction	17.4×10^{-2} (m)	"
P	reproductive period	365 (d)	[99]
J	time length of embryonic stage	51 (d)	[99, 103]
A_1	half saturation constant modulated by E_s	3.0×10^{-4} (g/egg)	created
a_2	energy to mobilize labile structure for eggs	2.0×10^{2} ($J \cdot g^{-1}$)	"
a_3	energy to mobilize labile lipid for eggs	2.0×10^{2} ($J \cdot g^{-1}$)	"

Table 3: The variables and parameters in the uptake model

Symbol	*Default value*	*Interpretation*	*Units*
Variables			
C_T		Toxicant concentration in whole fish	g/cm^3
C_w		Toxicant concentration in ambient water	g/cm^3
C_A		Toxicant concentration in aqueous portion of the fish	g/cm^3
C_F		Toxicant concentration in intestinal contents	g/cm^3
S_g		Active exposure area	cm^2
F		Weight of ingested food per day	g/d
E		Weight of material defecated per day	g/d
V		Volume of the organism	cm^3
W_T		Weight of the organism	g
P_A		Fraction of fish that is aqueous	nondim.
P_L		Fraction of fish that is lipid	nondim.
P_S		Fraction of fish that is structure	nondim.
Parameters			
k_w	530	Conductivity:exposure	cm^2/d
k_E	0.2	Partition coefficient of chemical to excrement	nondim.
K_L	1	Lipid/water partition coefficient	nondim.
K_S	0.2	Structure/water partition coefficient	nondim.

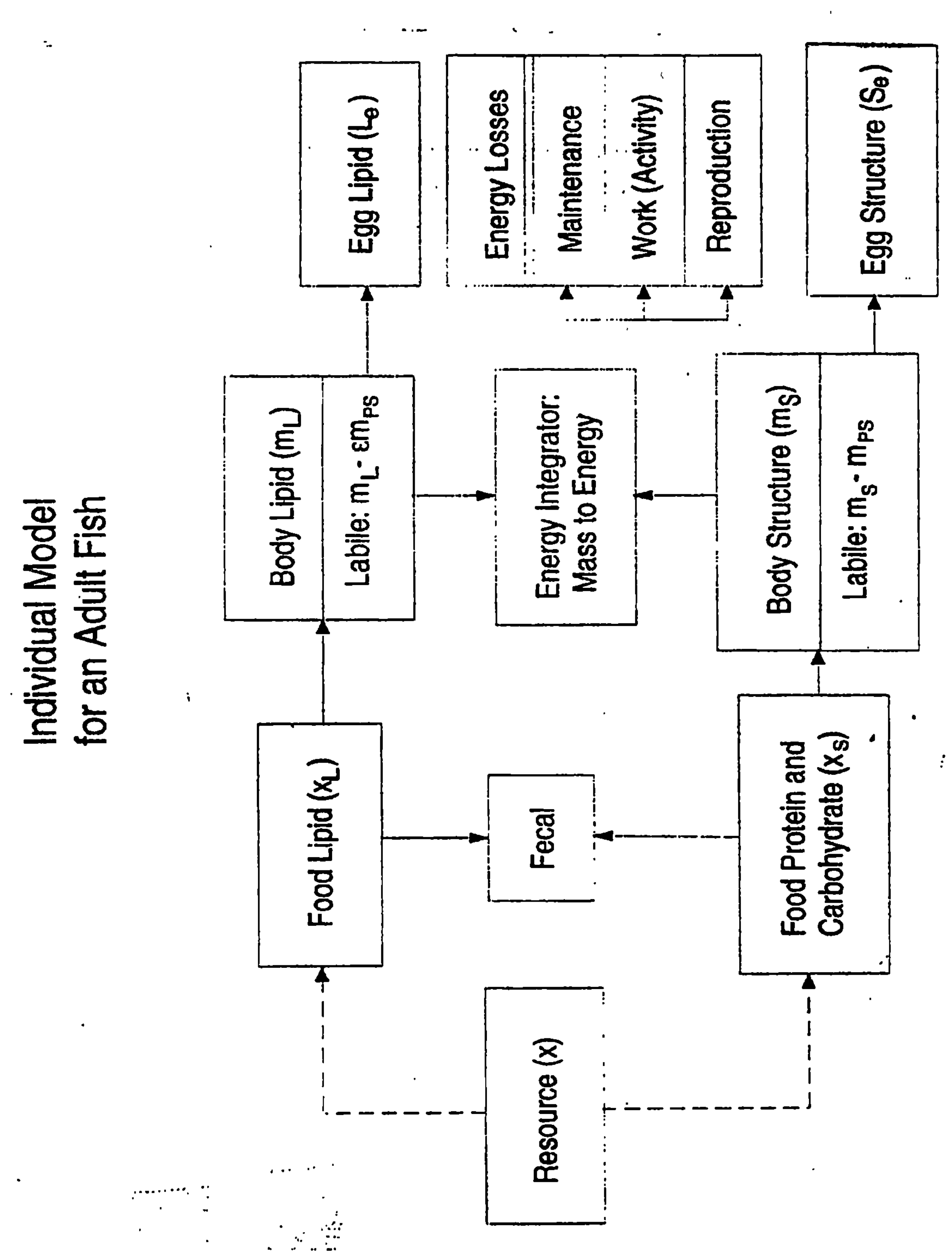


Figure 1: Individual Based Adult Fish Model

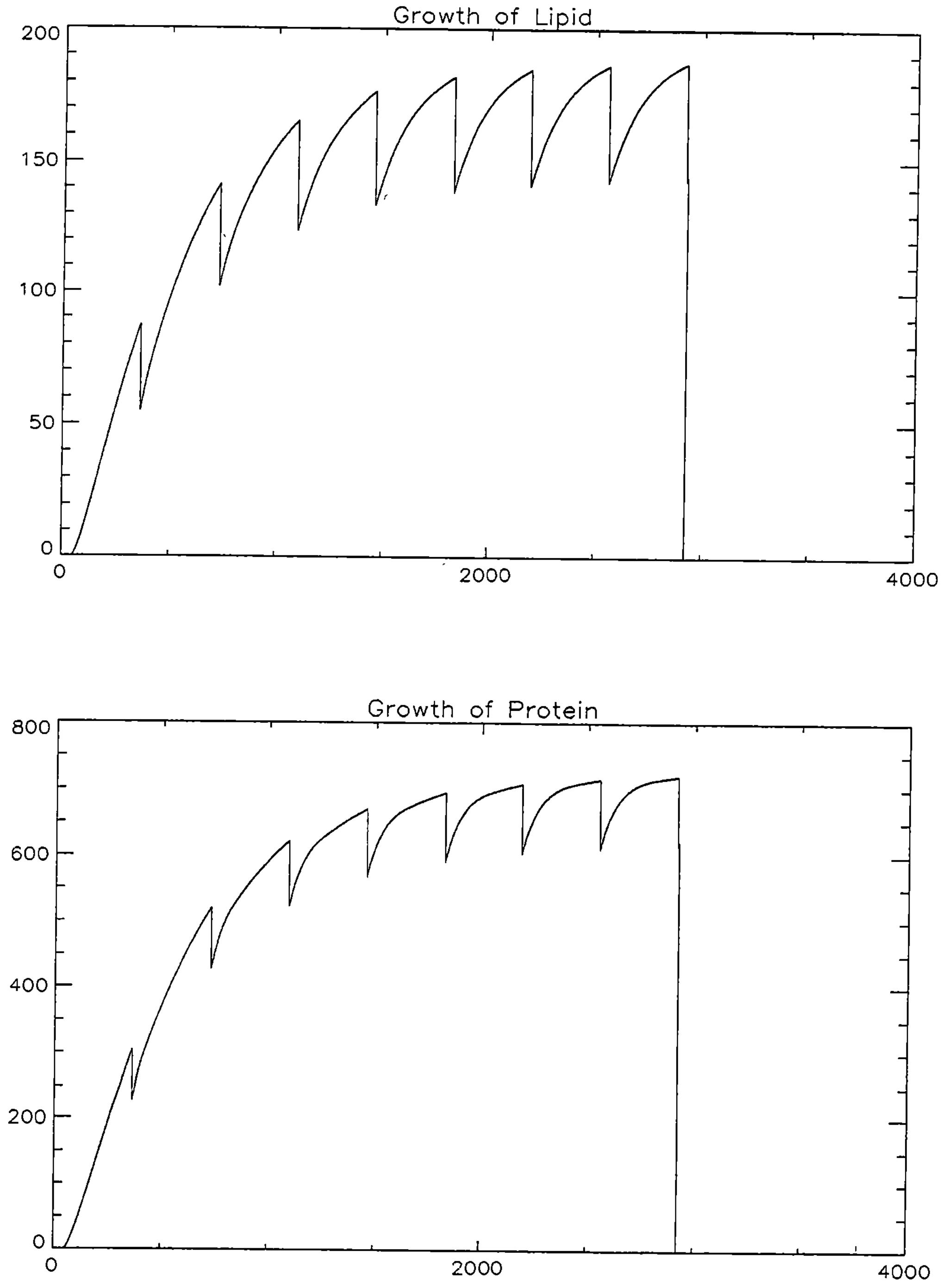
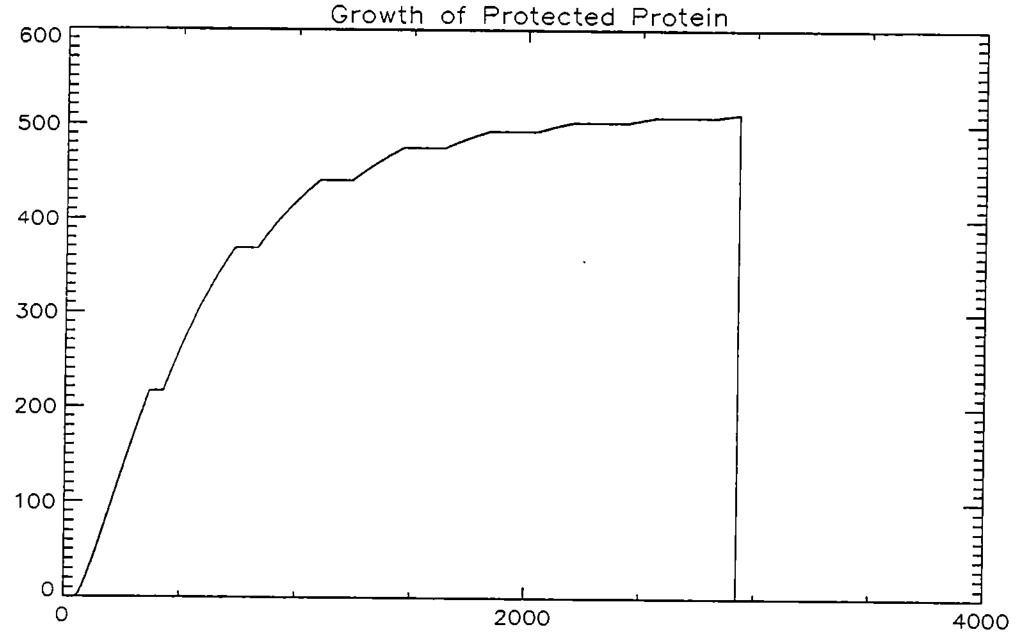


Figure 2: Individual Fish Growth (1)



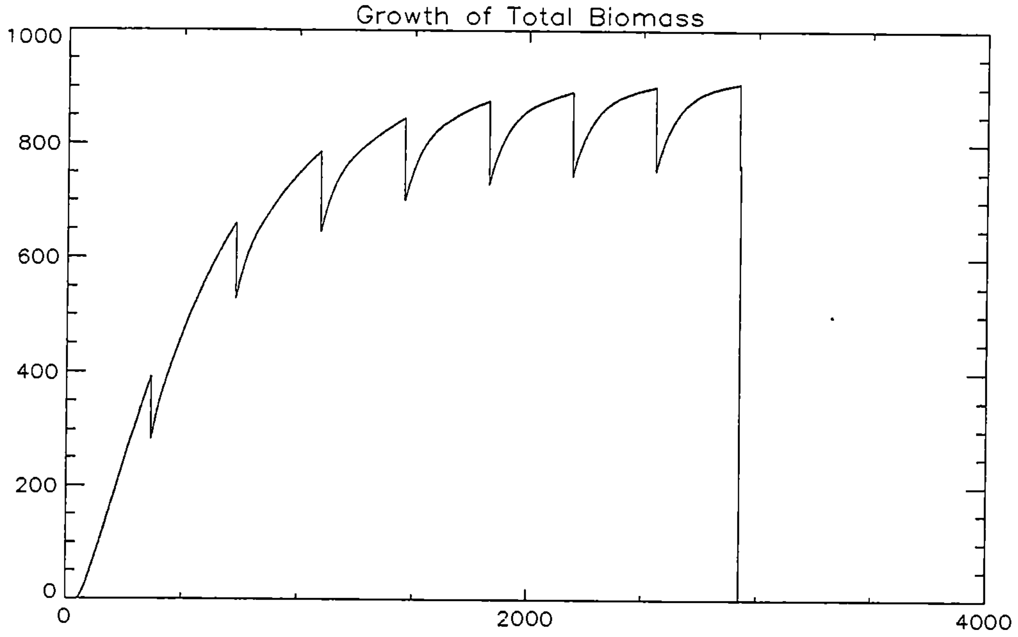


Figure 3: Individual Fish Growth (2)

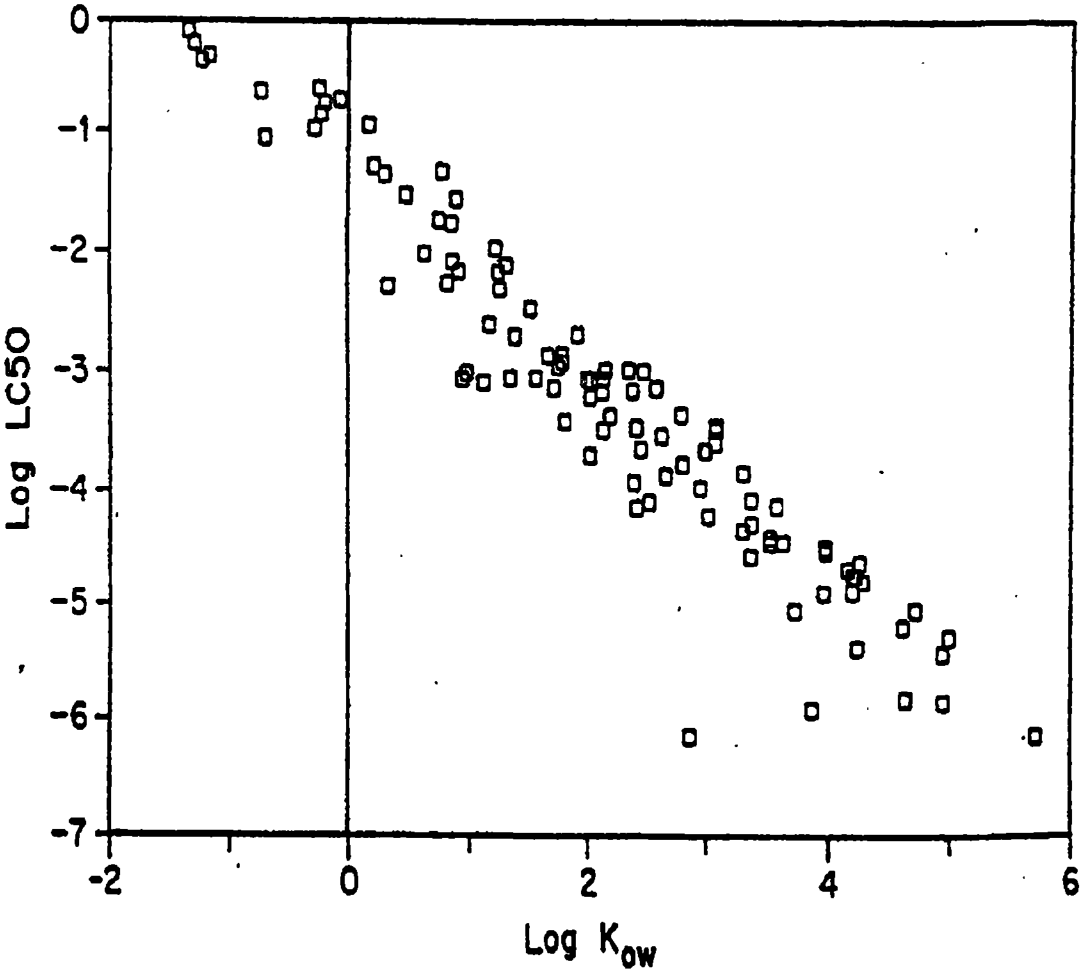


Figure 4: Relationship between $\log LC_{50}$ and $\log K_{ow}$

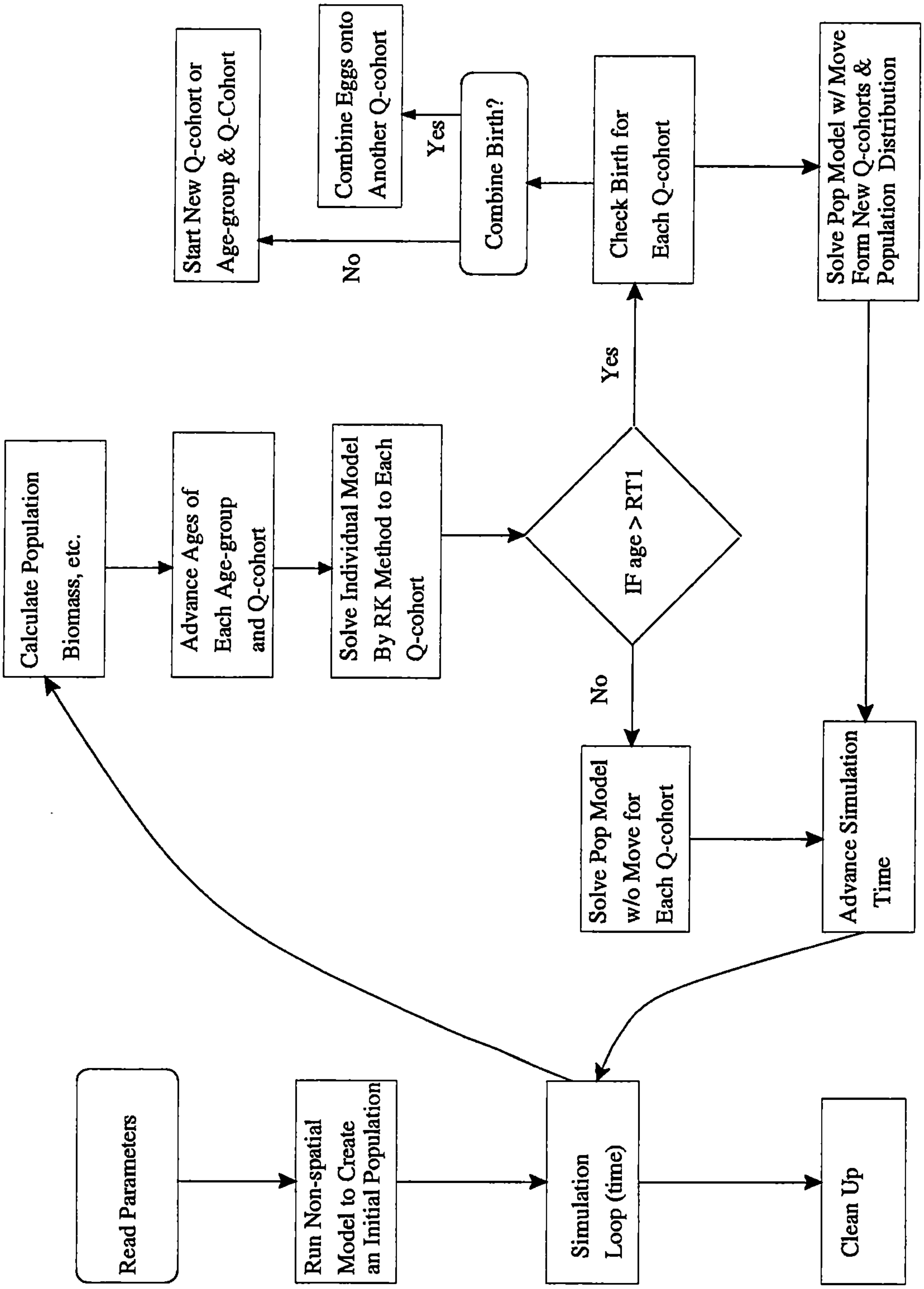


Figure 5: Flow Chart for Computational Model

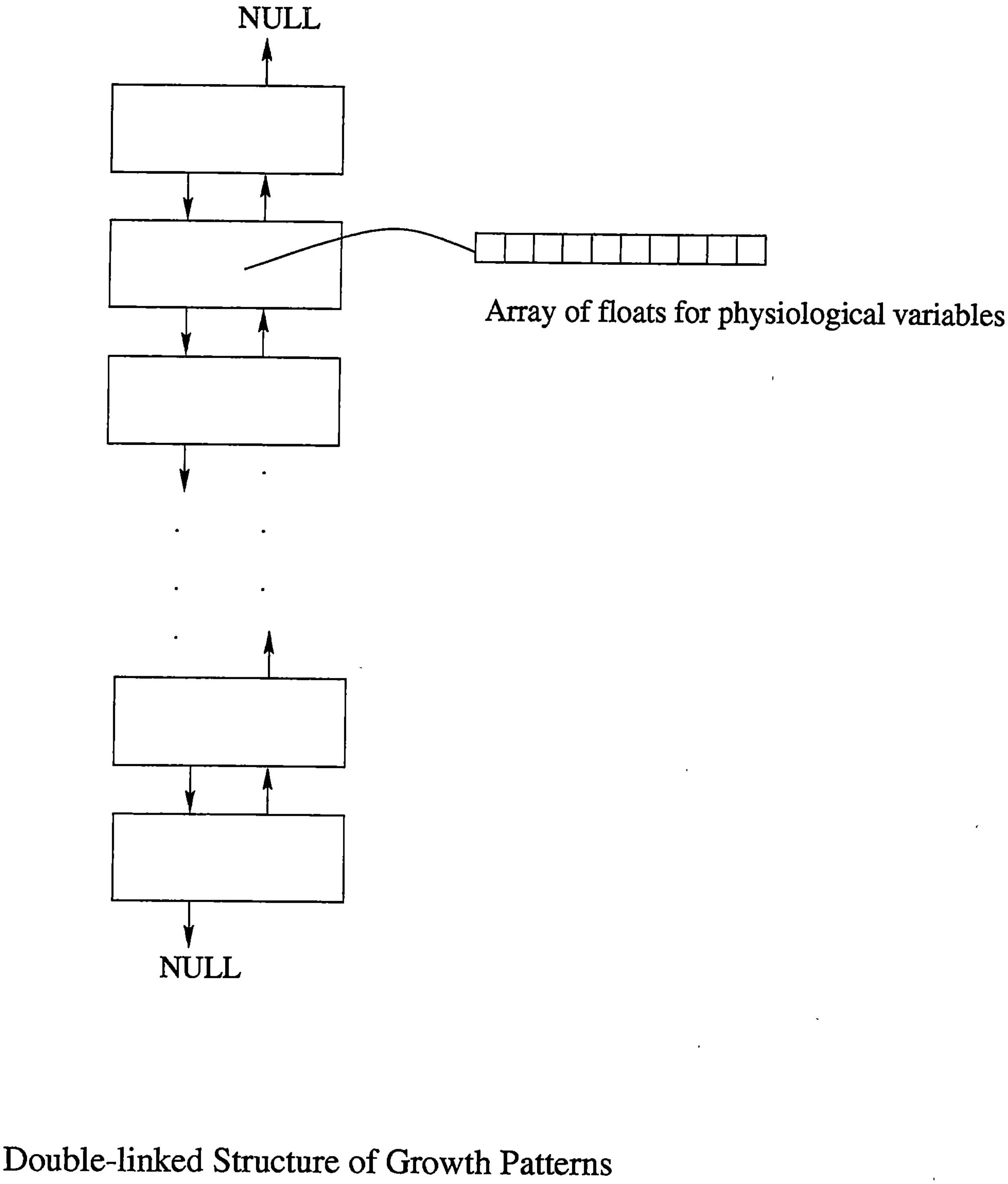


Figure 6: Double Linked List of *q-cohort*

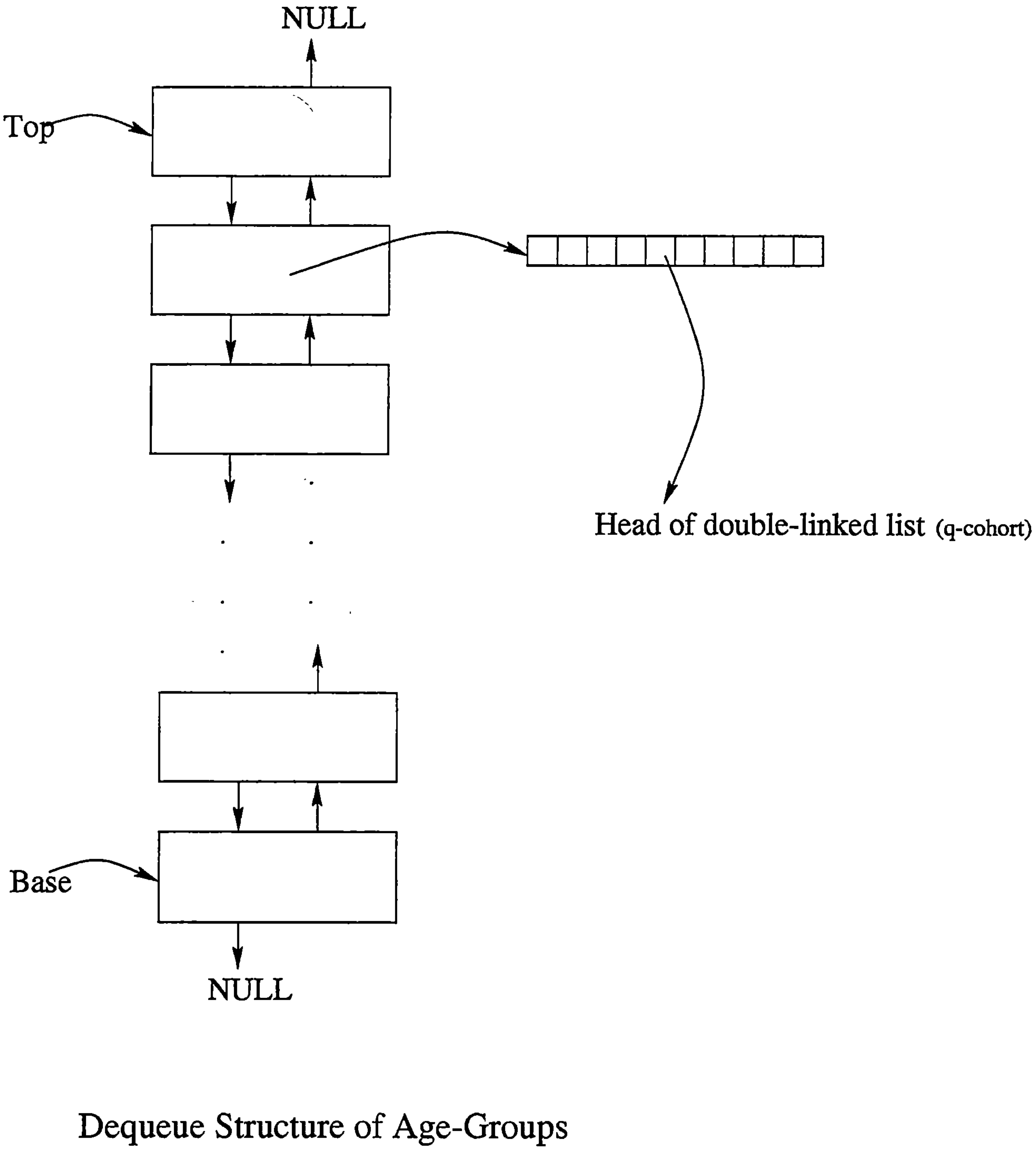


Figure 7: Dequeue Structure of *Age-Group*

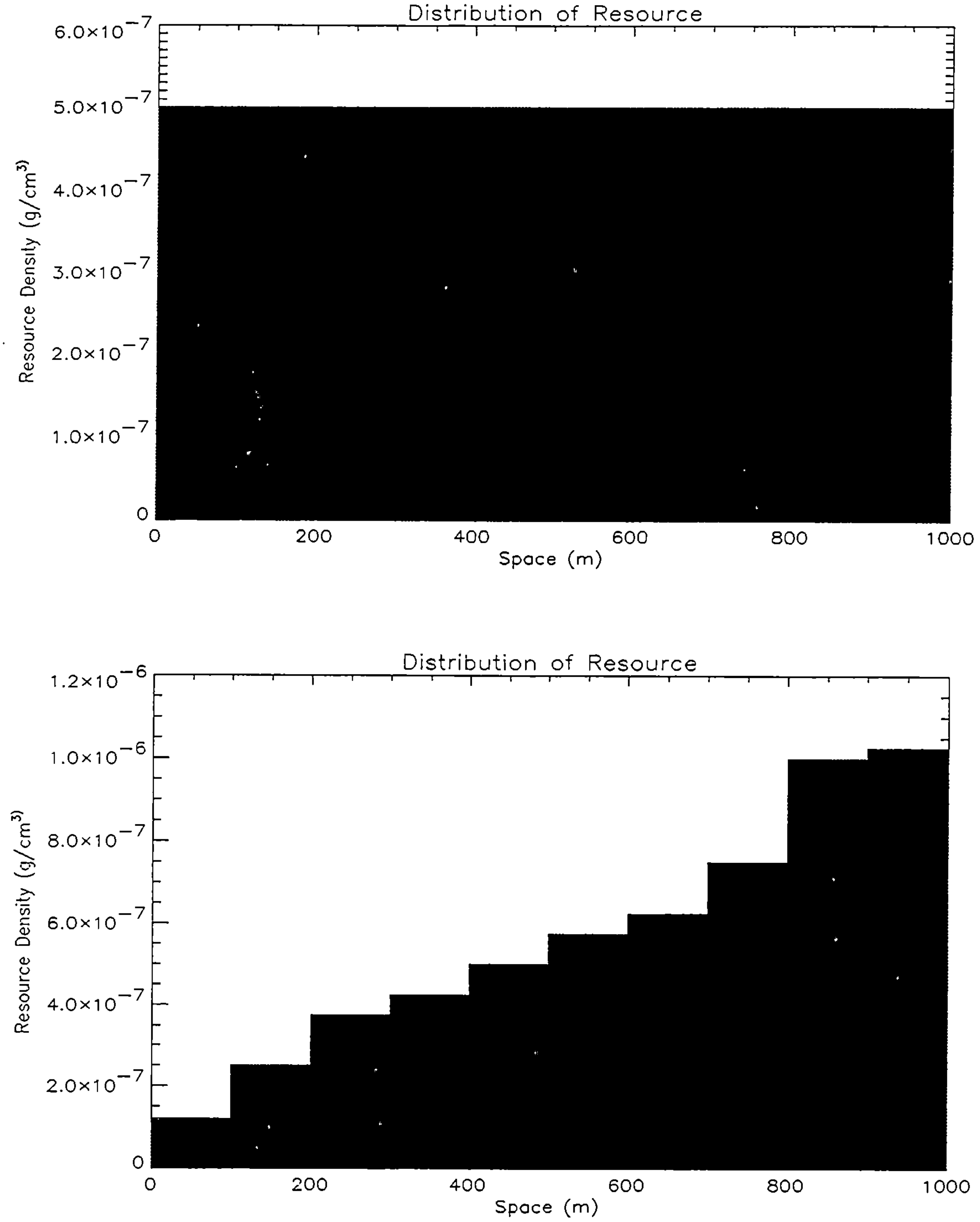


Figure 8: Resource Distribution Patterns

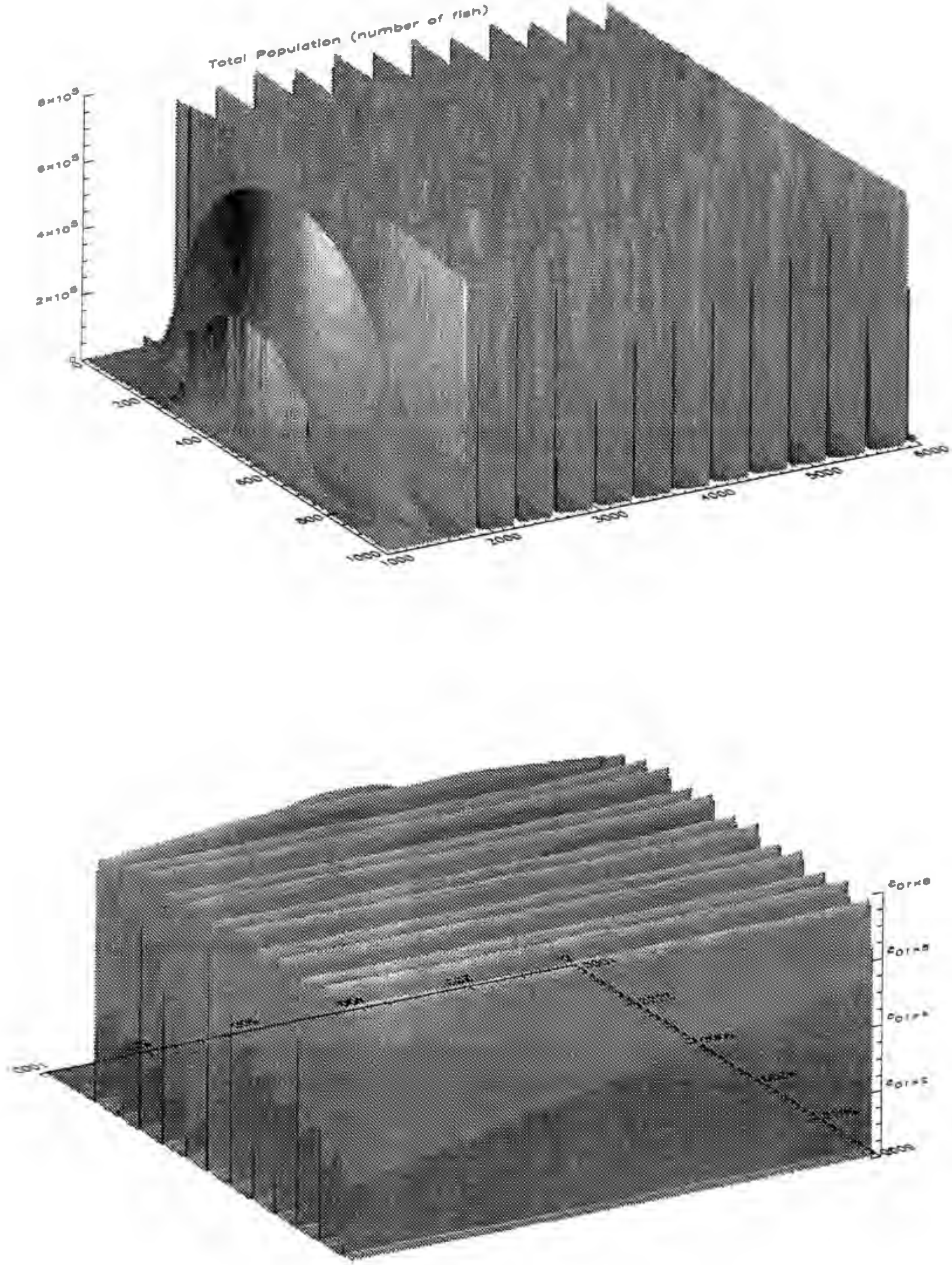


Figure 9: Total Fish Number of *Case 4.1*

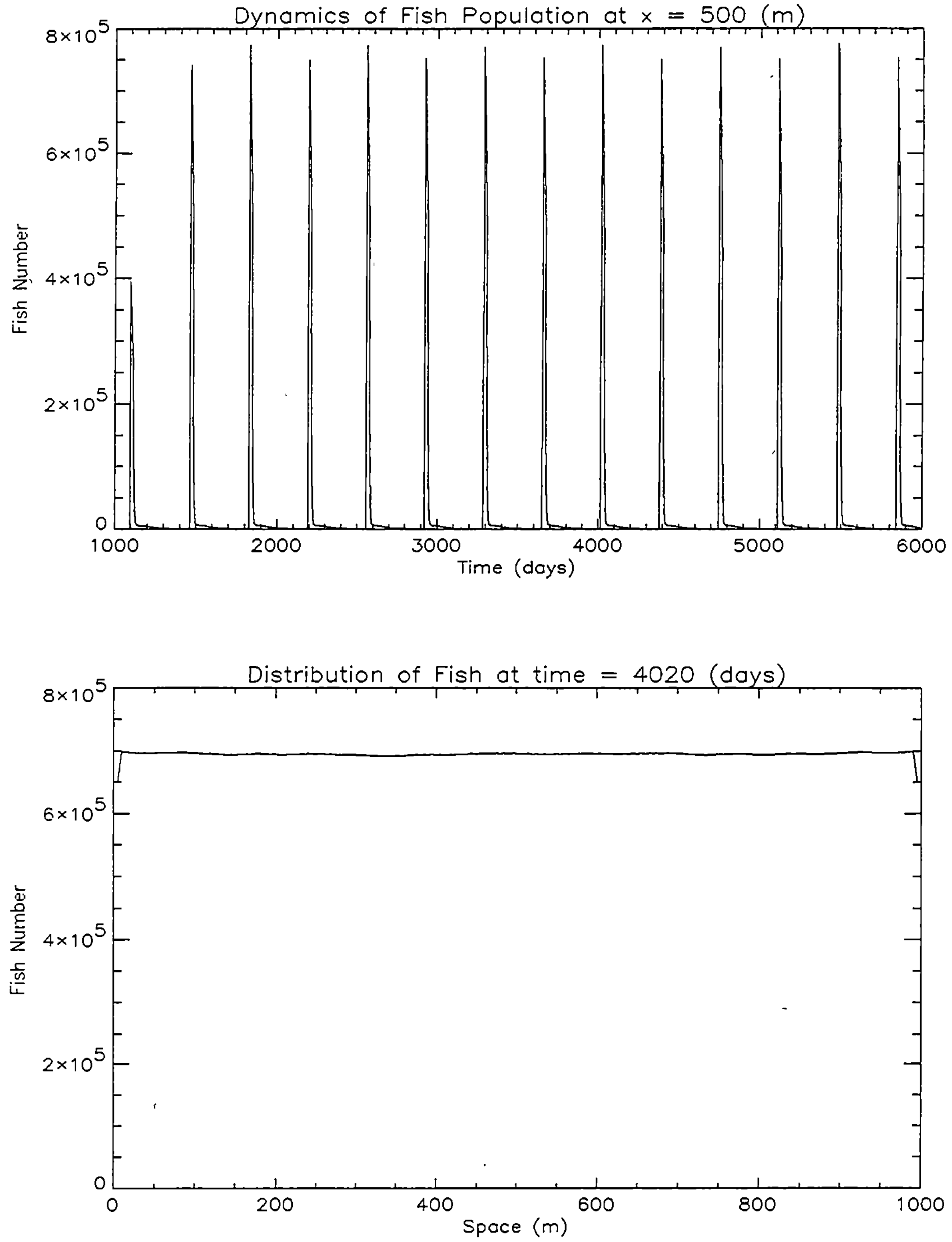


Figure 10: Population Dynamics/Distribution at a Location/Time of *Case 4.1*

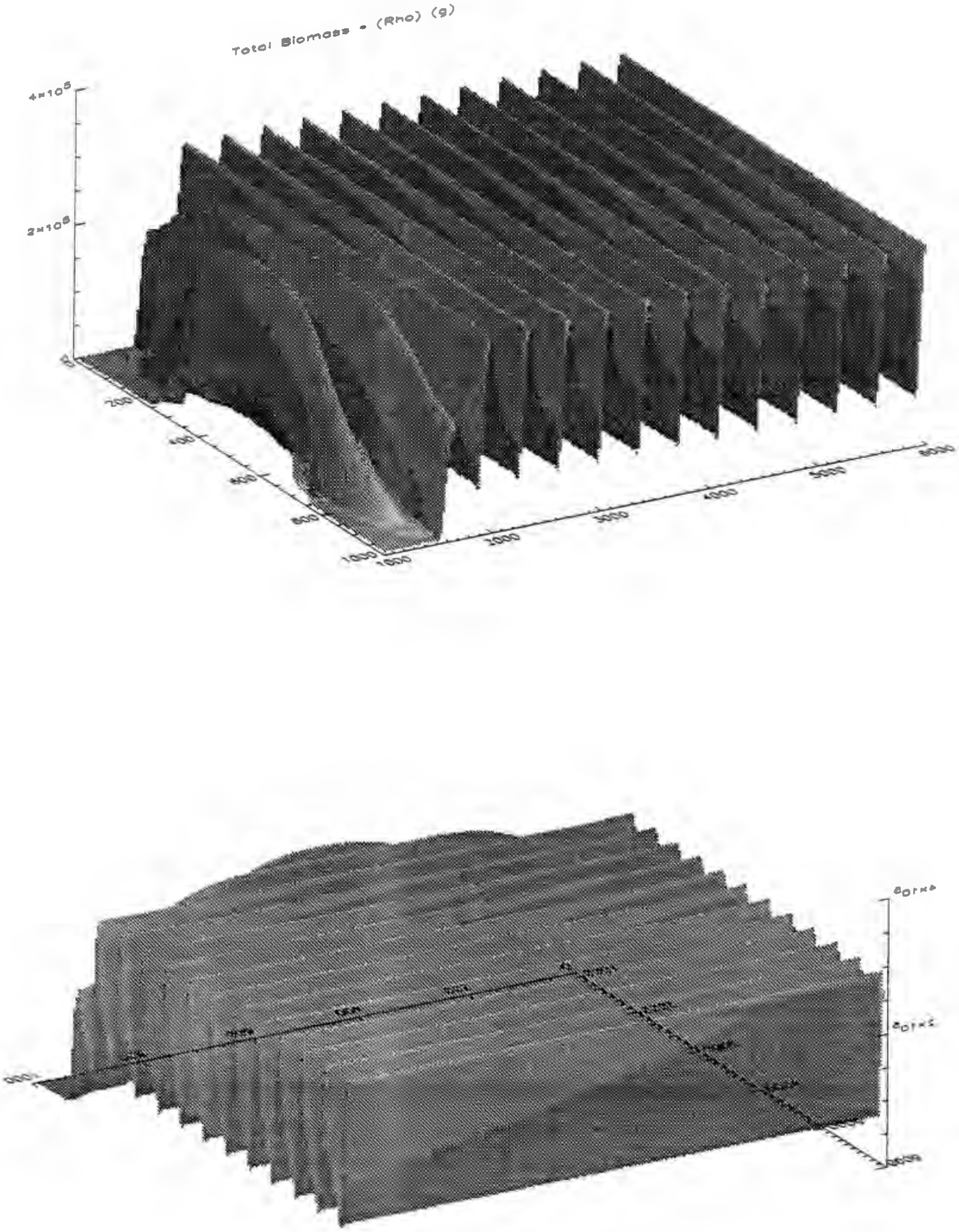


Figure 11: Total Biomass Distribution of *Case 4.1*

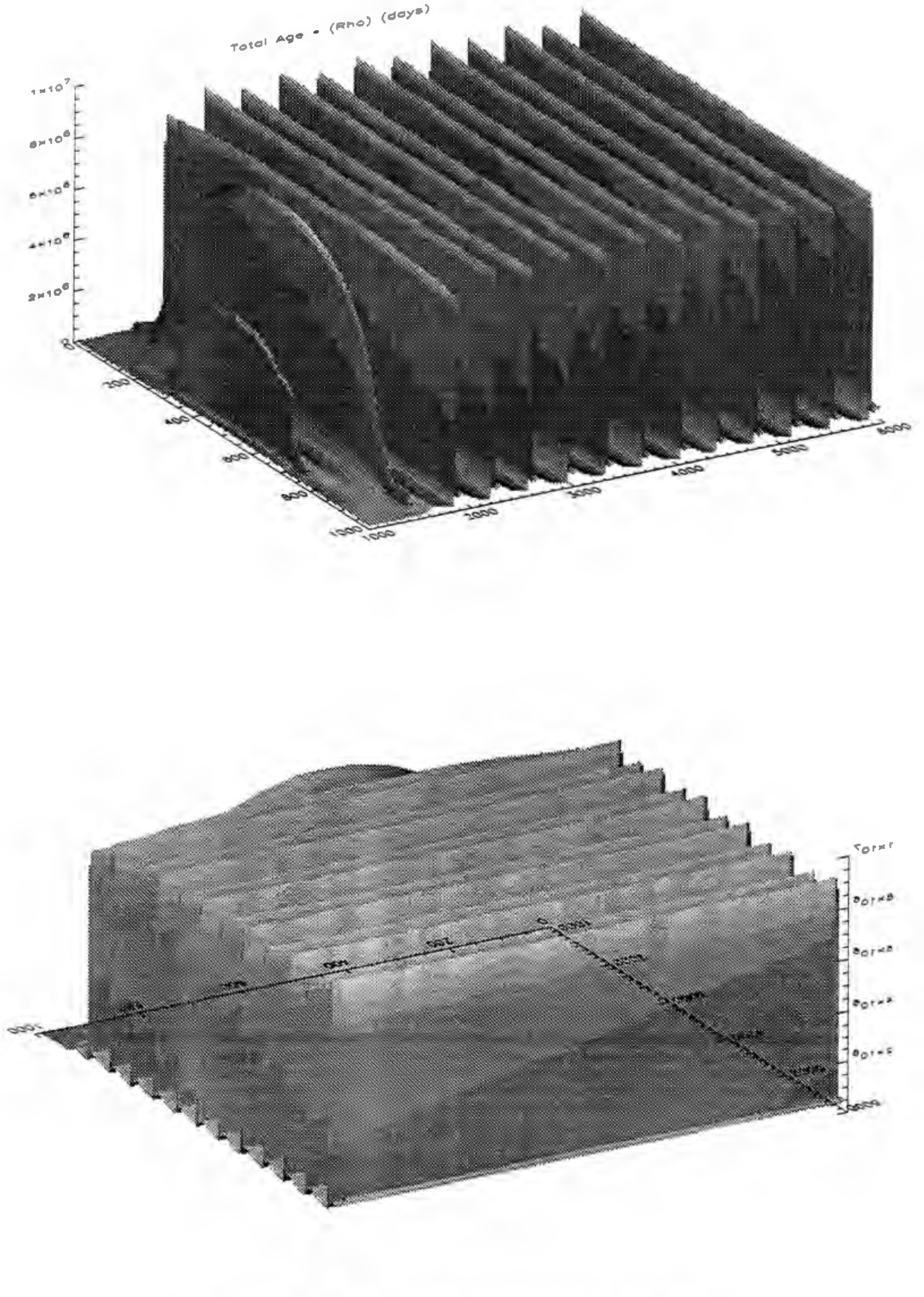


Figure 12: Total Age Distribution of *Case 4.1*

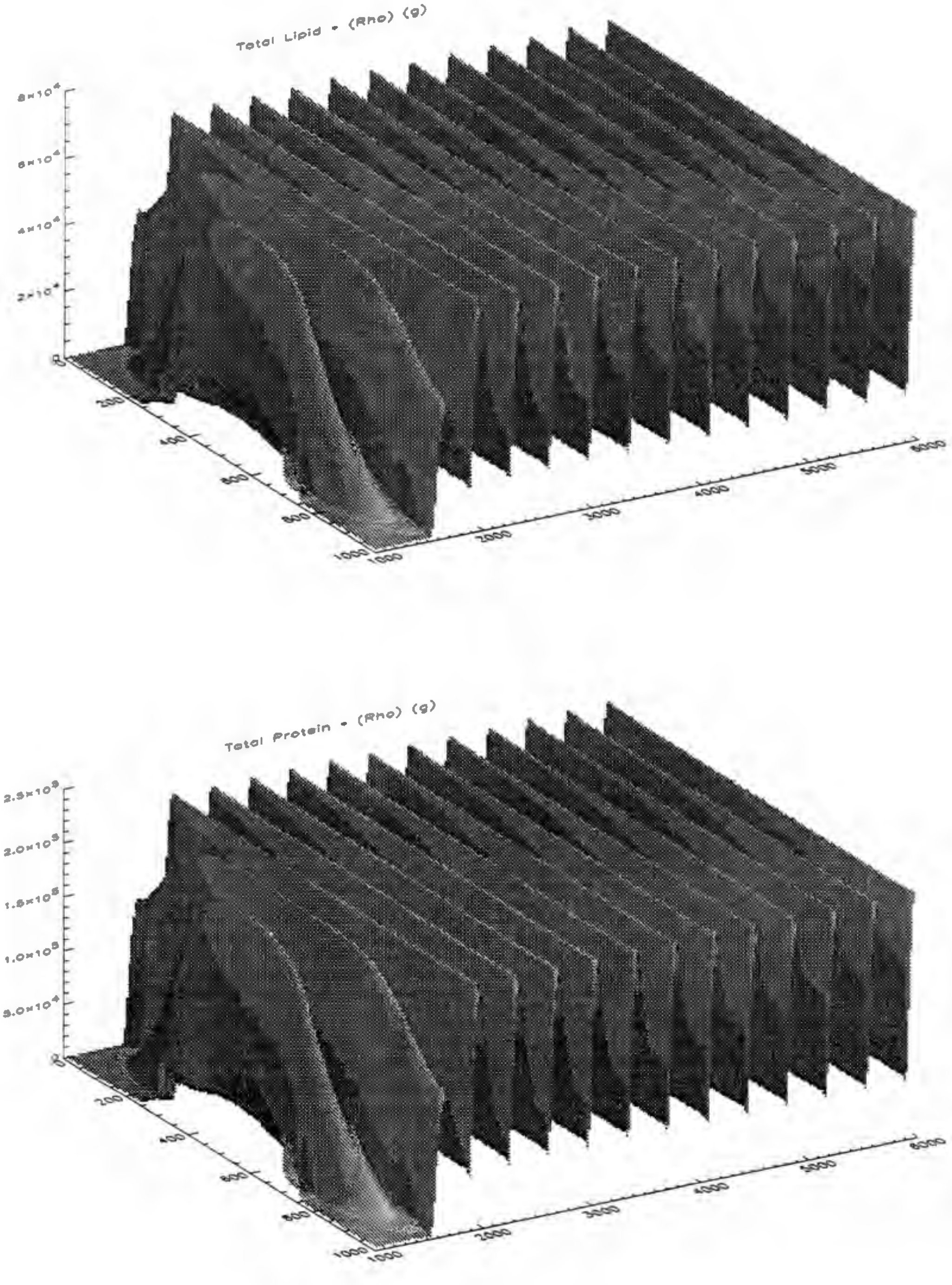


Figure 13: Total Lipid and Protein Distribution of *Case 4.1*

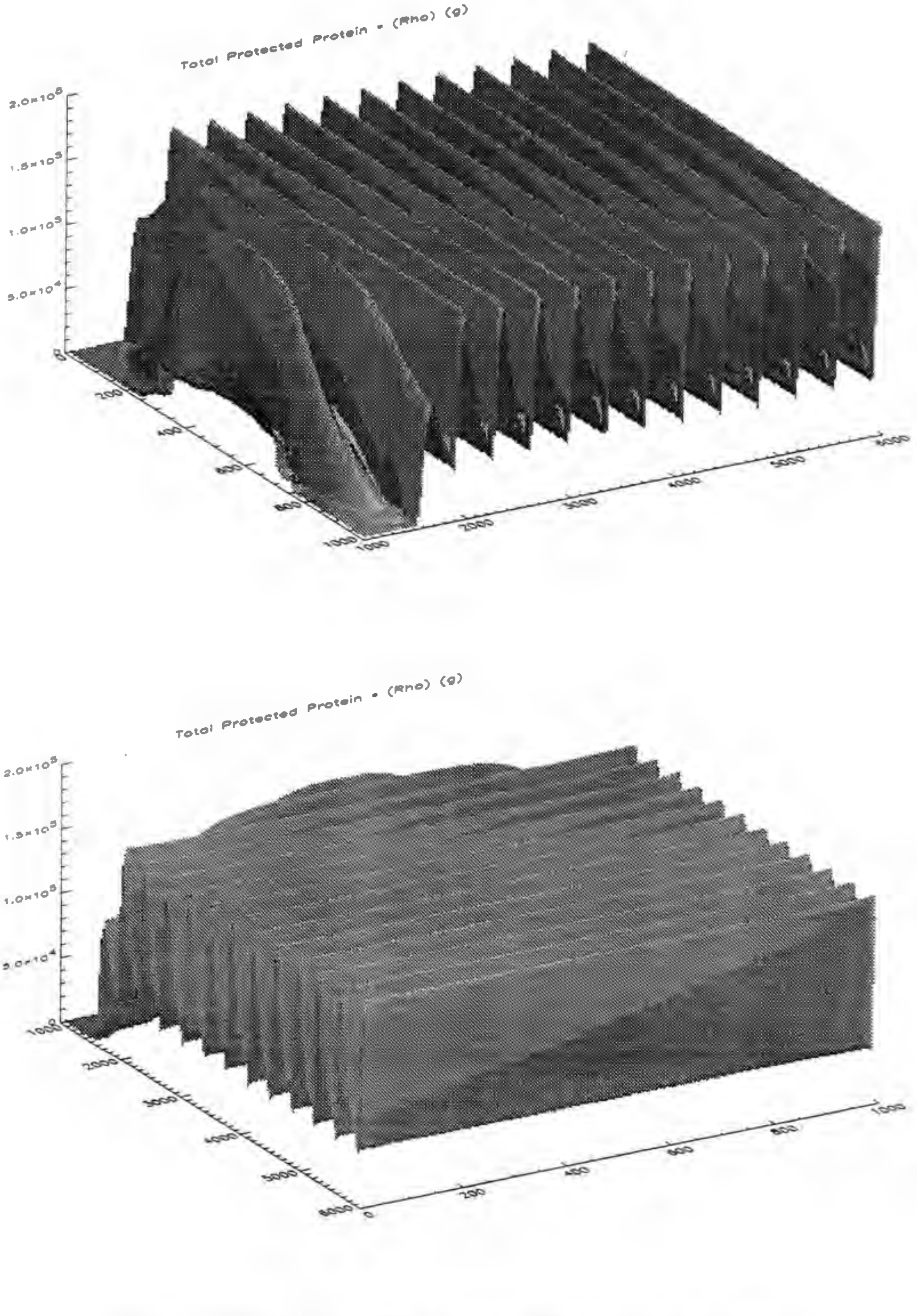


Figure 14: Total Protected Protein Distribution of *Case 4.1*

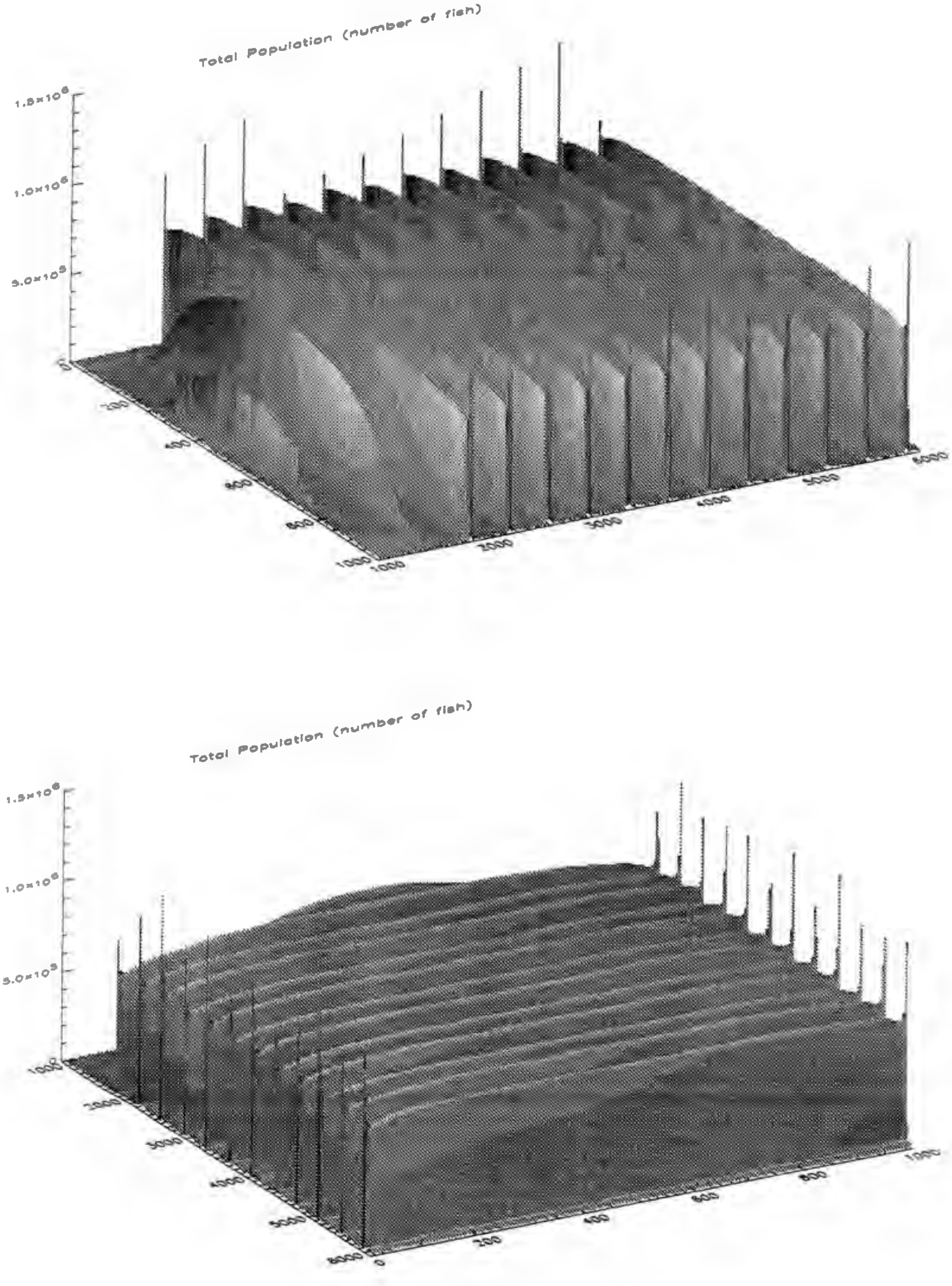


Figure 15: Total Fish Number of *Case 4.2*

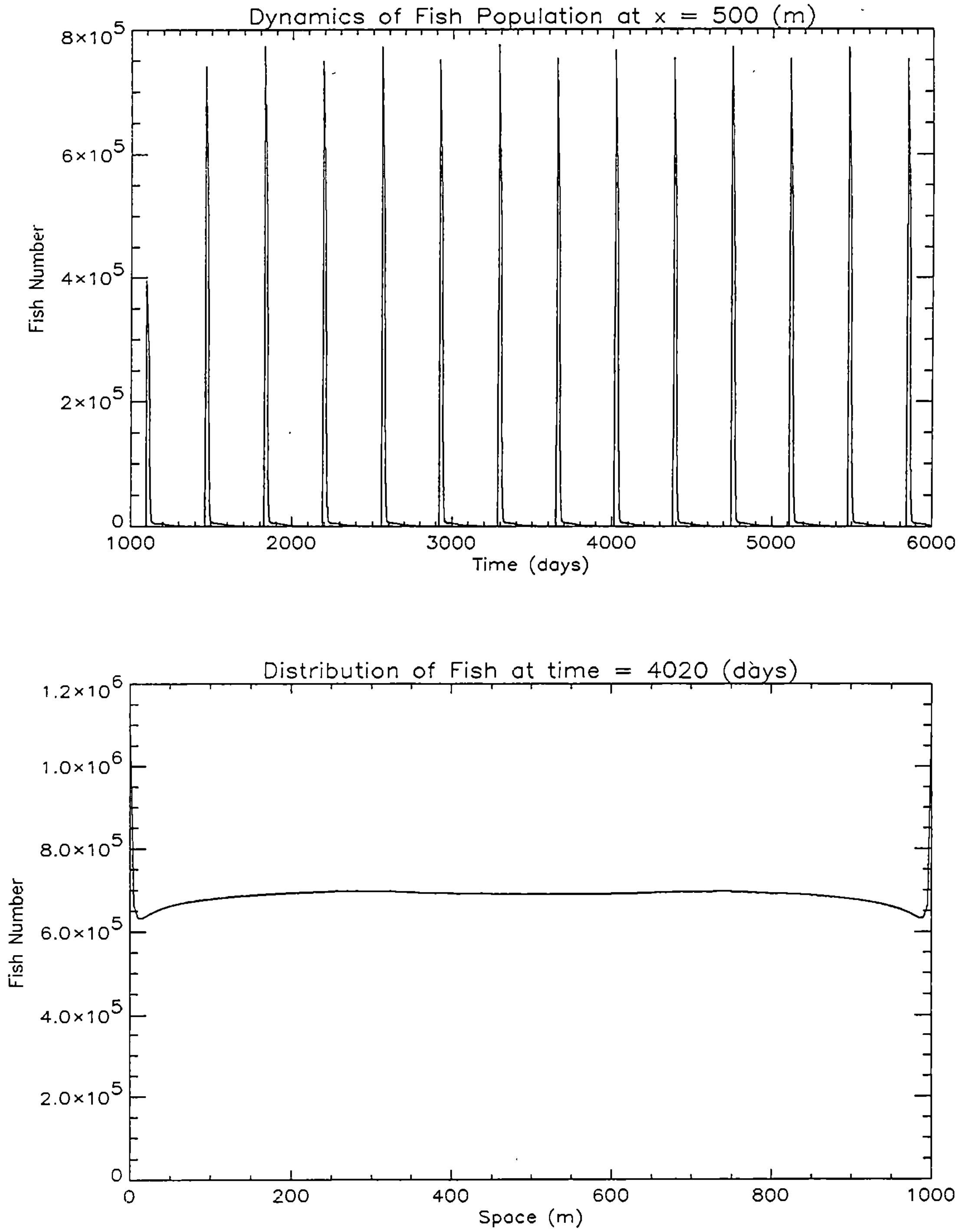


Figure 16: Population Dynamics/Distribution at a Location/Time of *Case 4.2*

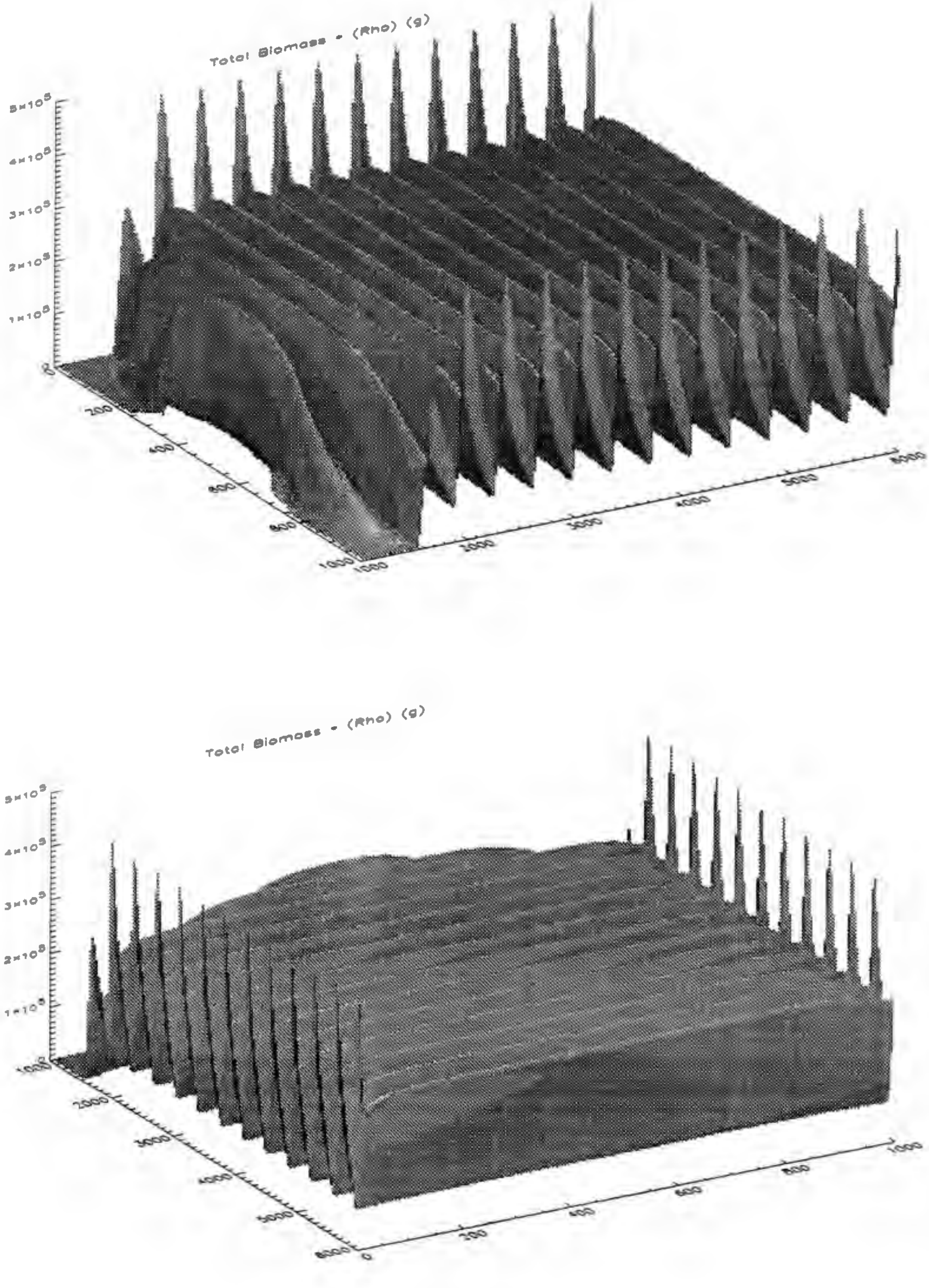


Figure 17: Total Biomass Distribution of *Case 4.2*

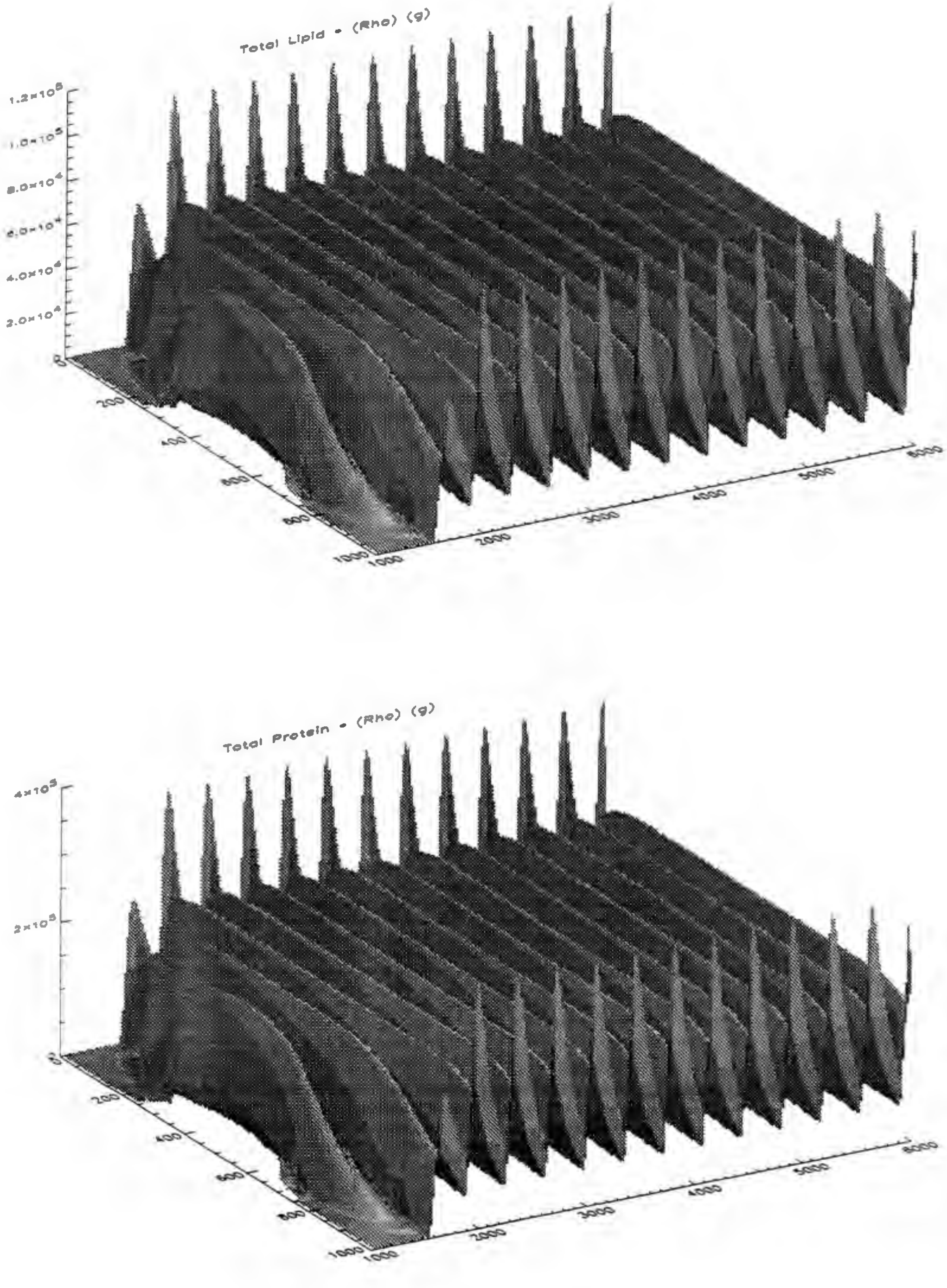


Figure 18: Total Lipid and Protein Distribution of *Case 4.2*

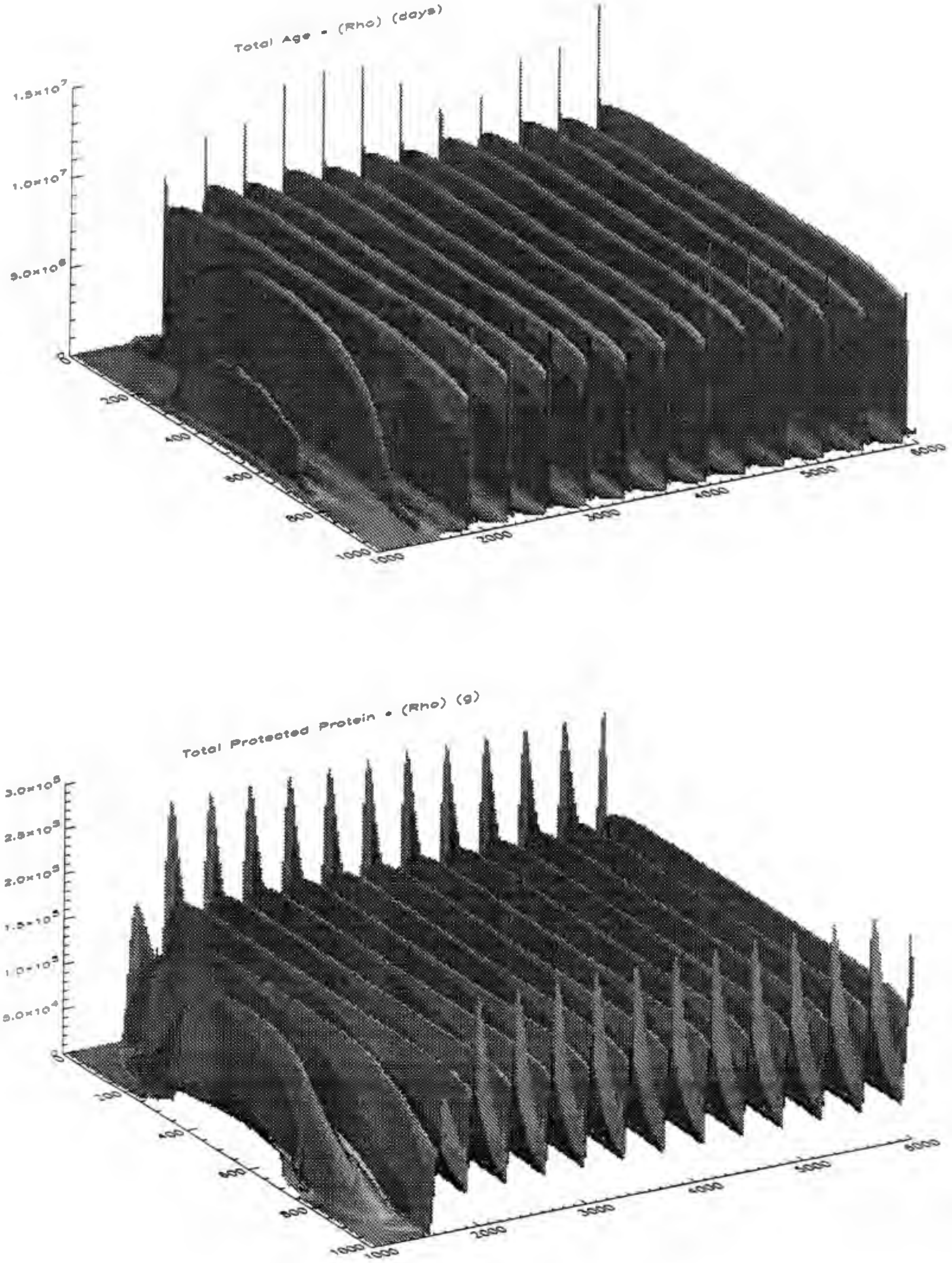


Figure 19: Total Age and Protected Protein Distribution of *Case 4.2*

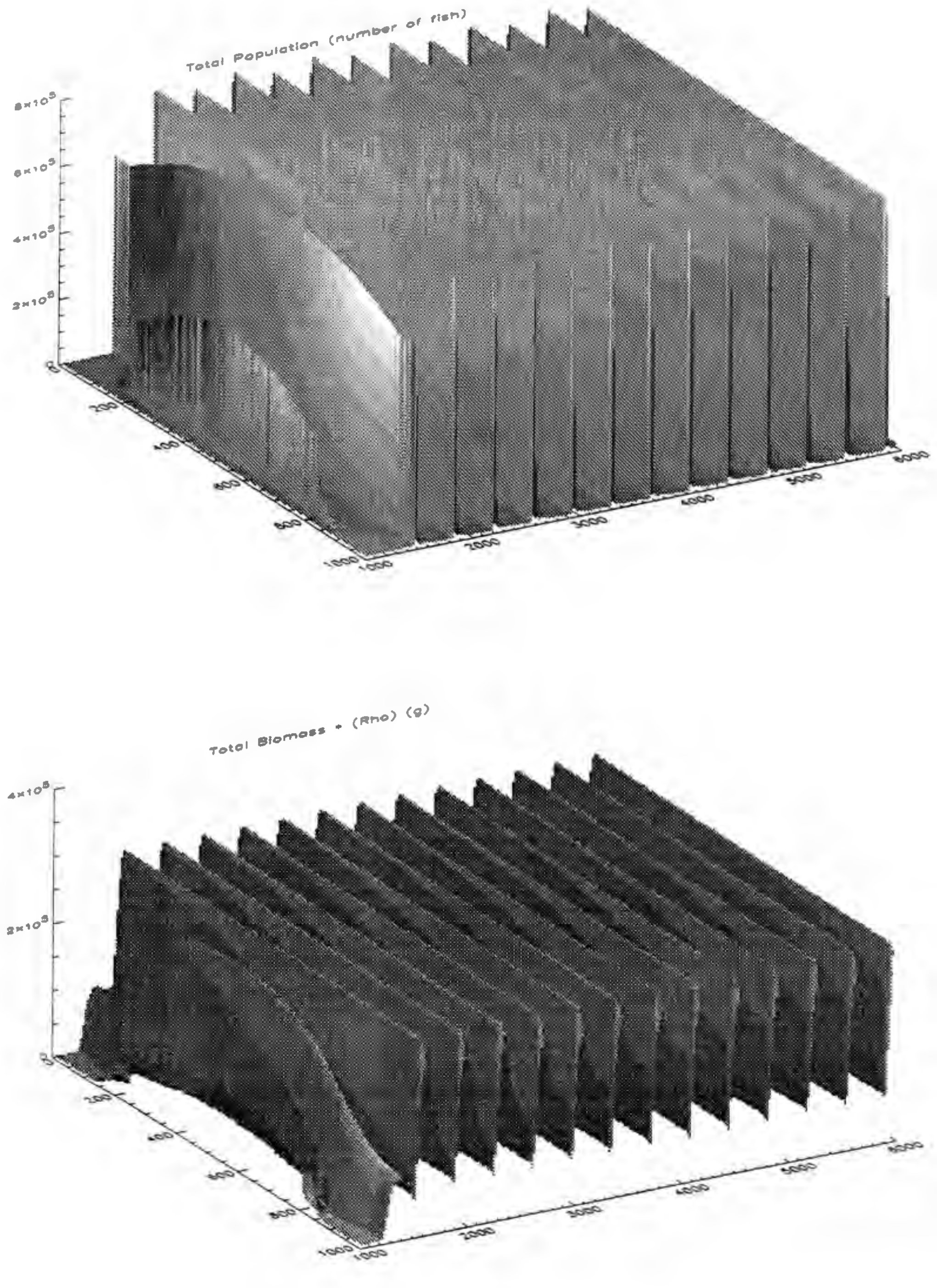


Figure 20: Total Fish Number and Biomass Distribution of *case 4.3*

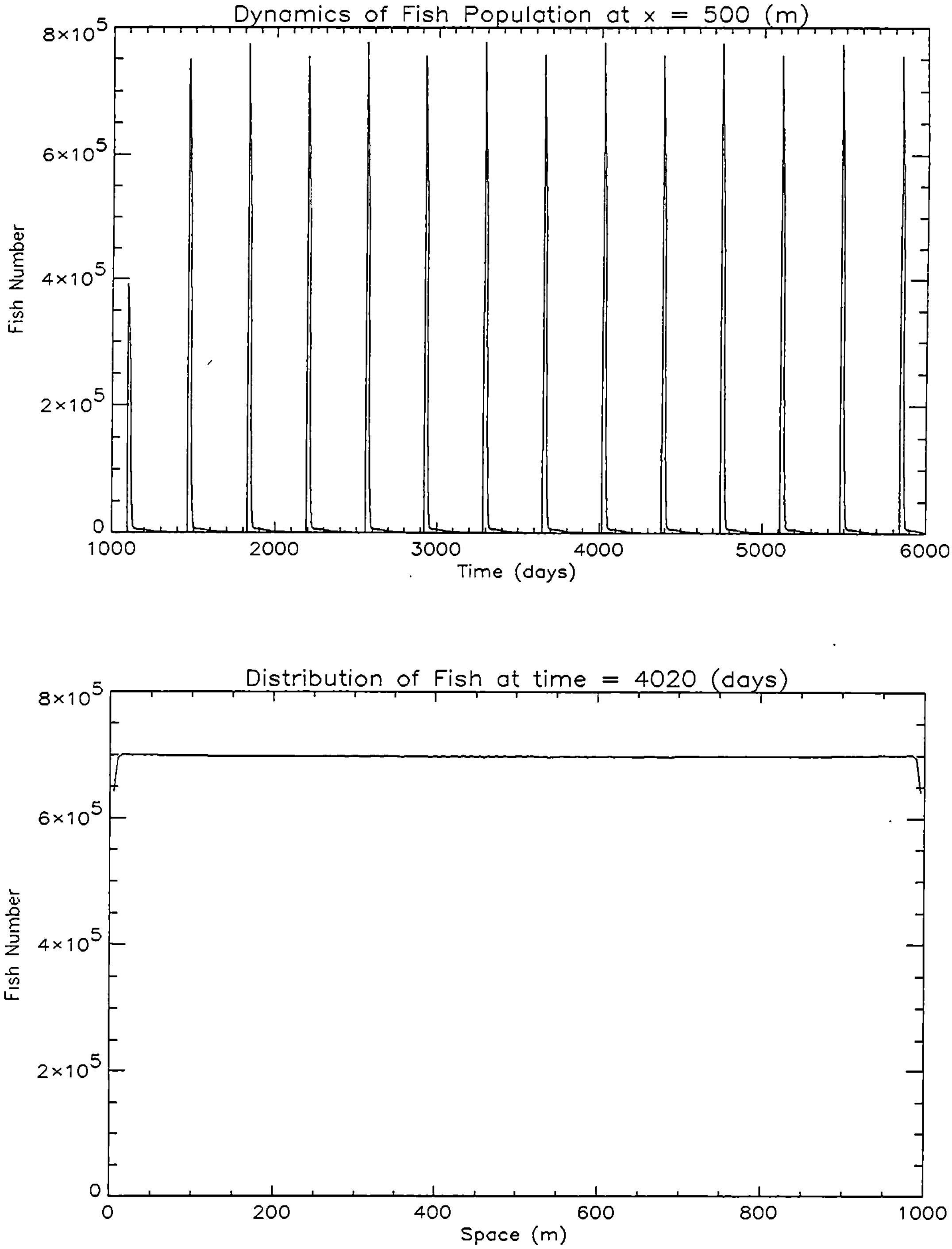


Figure 21: Population Dynamics/Distribution at a Location/Time of *Case 4.3*

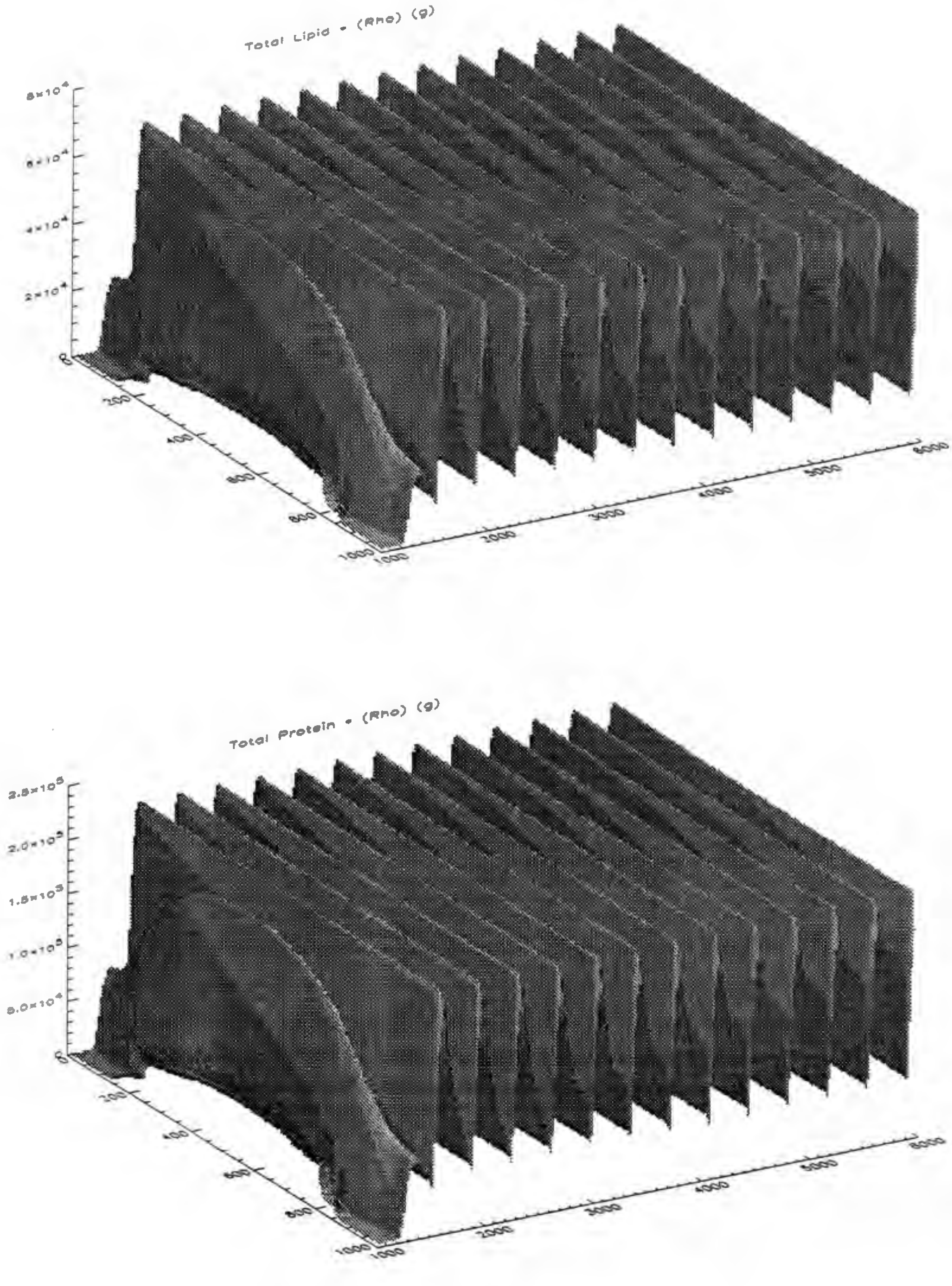


Figure 22: Total Lipid and Protein Distribution of *Case 4.3*

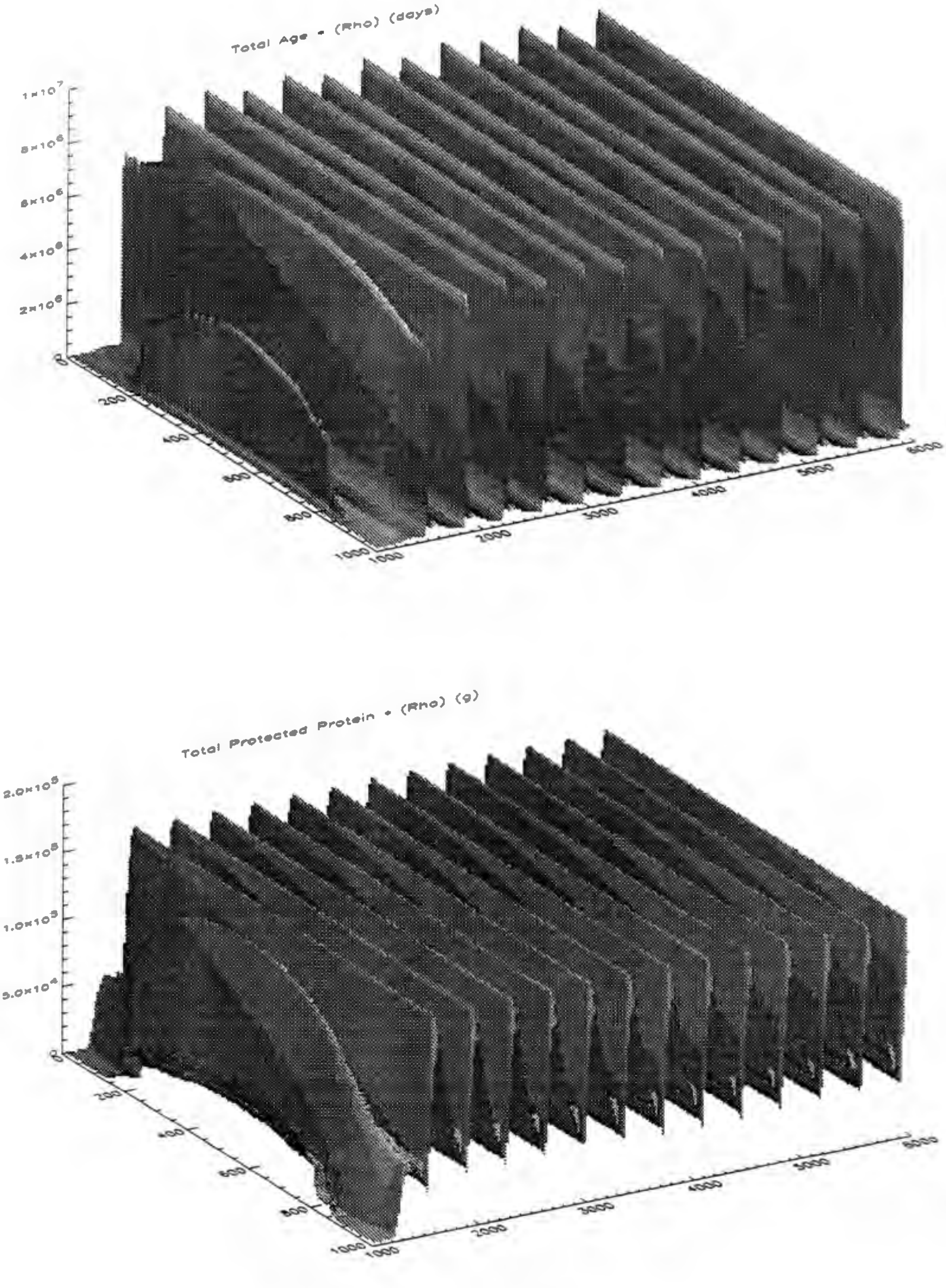


Figure 23: Total Age and Protected Protein Distribution of *Case 4.3*

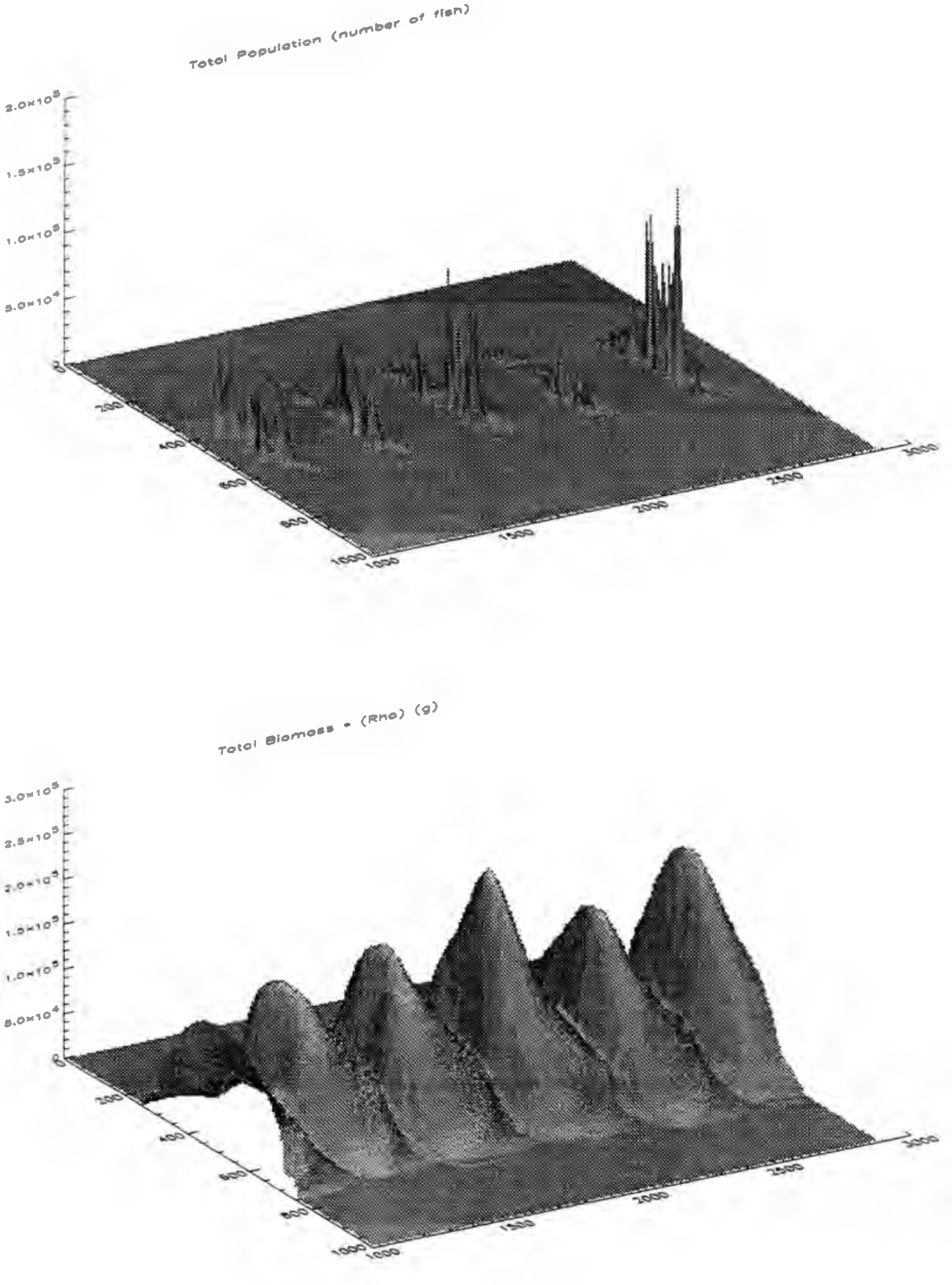


Figure 24: Total Fish number and Biomass Distribution of *Case 4.4*

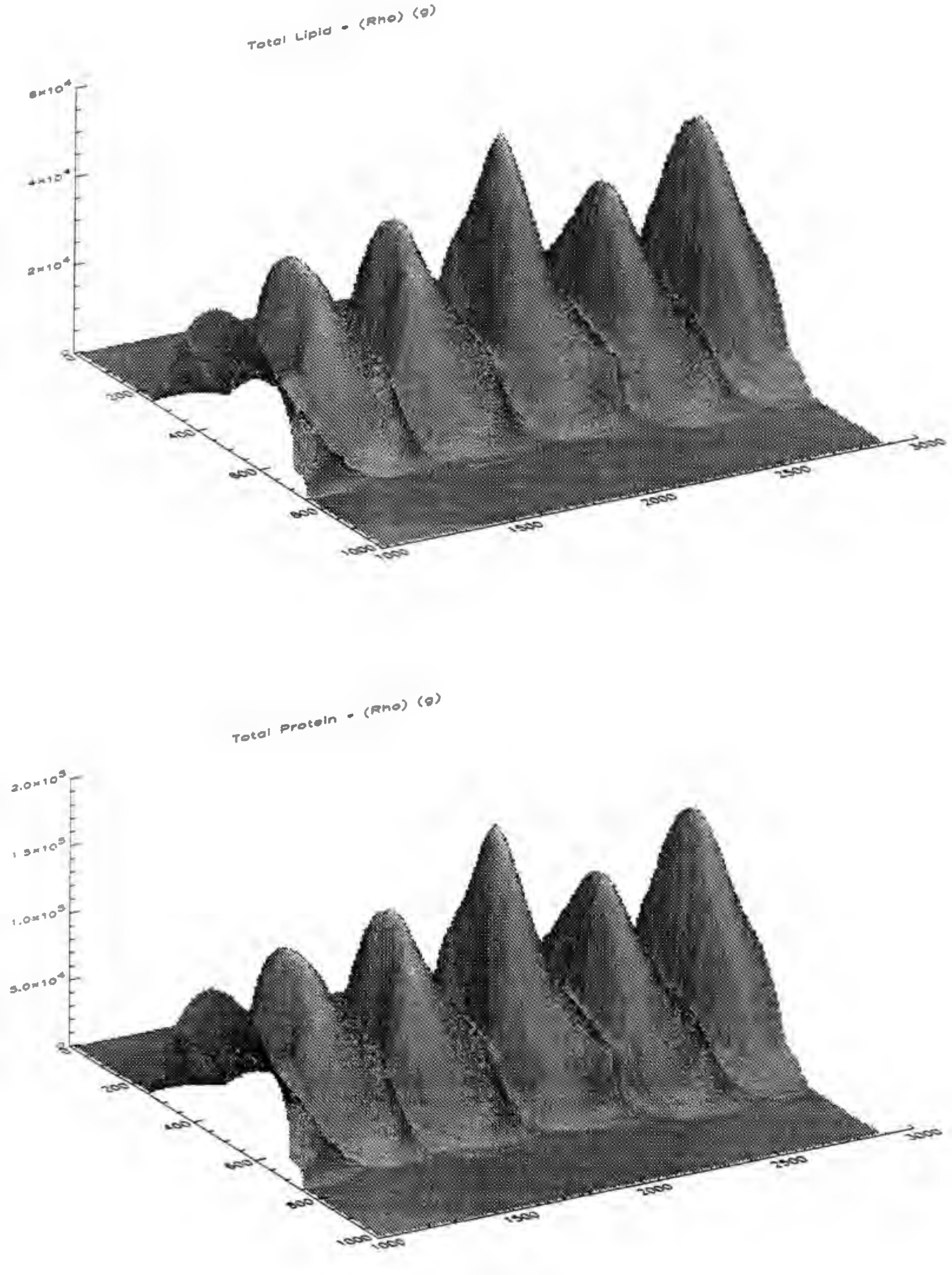


Figure 25: Total Lipid and Protein Distribution of *Case 4.4*

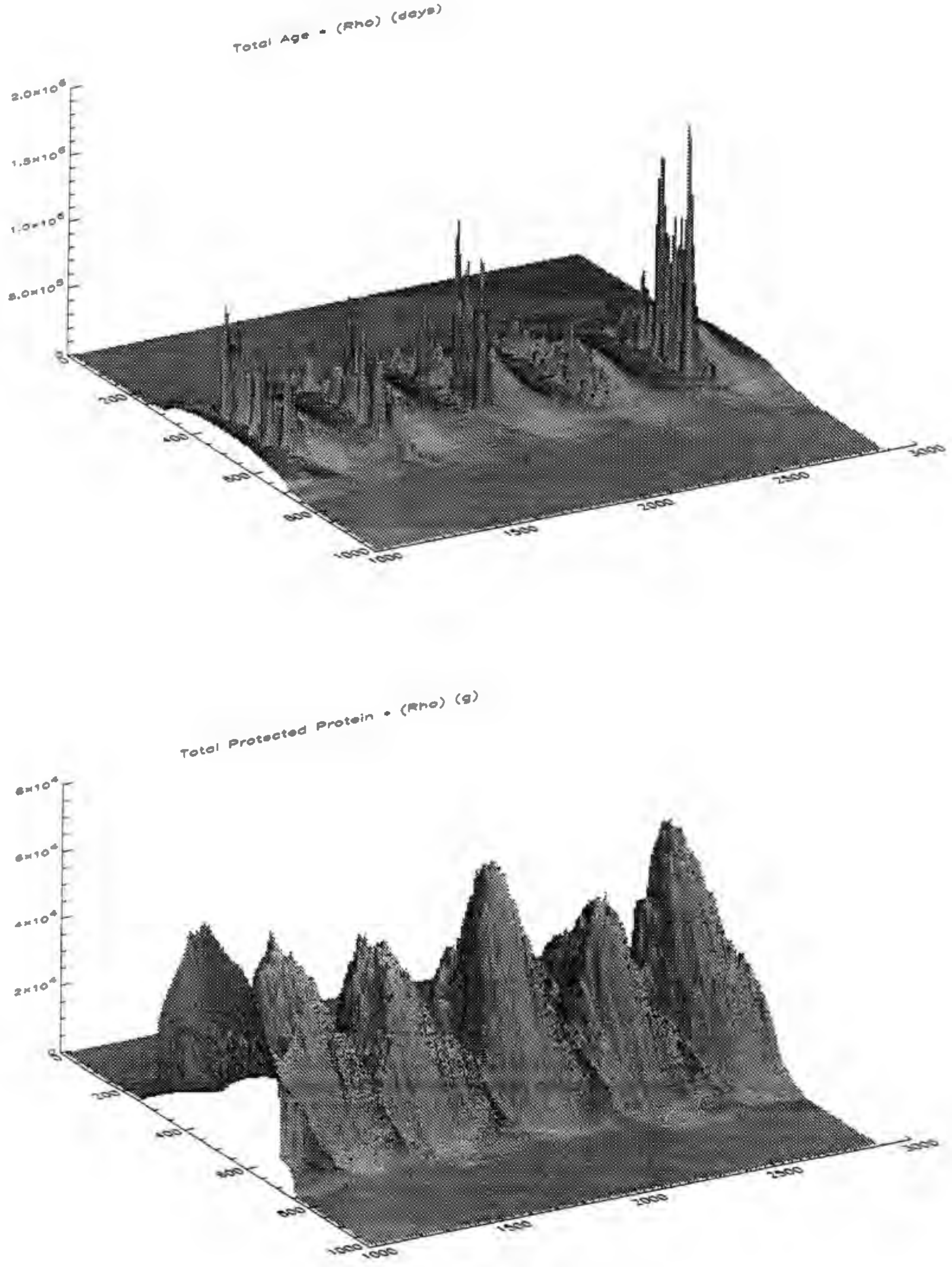


Figure 26: Total Age and Protected Protein Distribution of *Case 4.4*

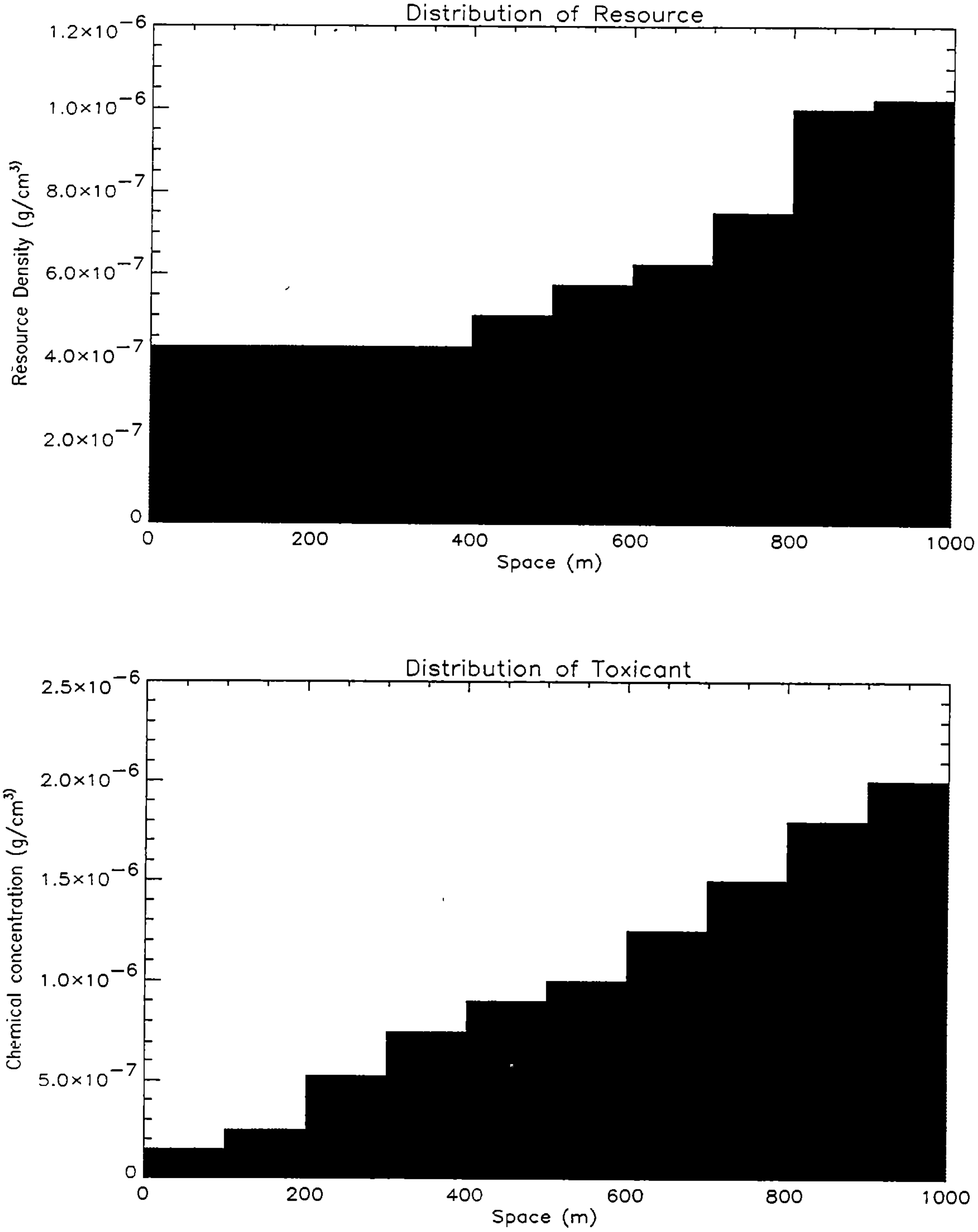


Figure 27: Resource and Chemical Distribution

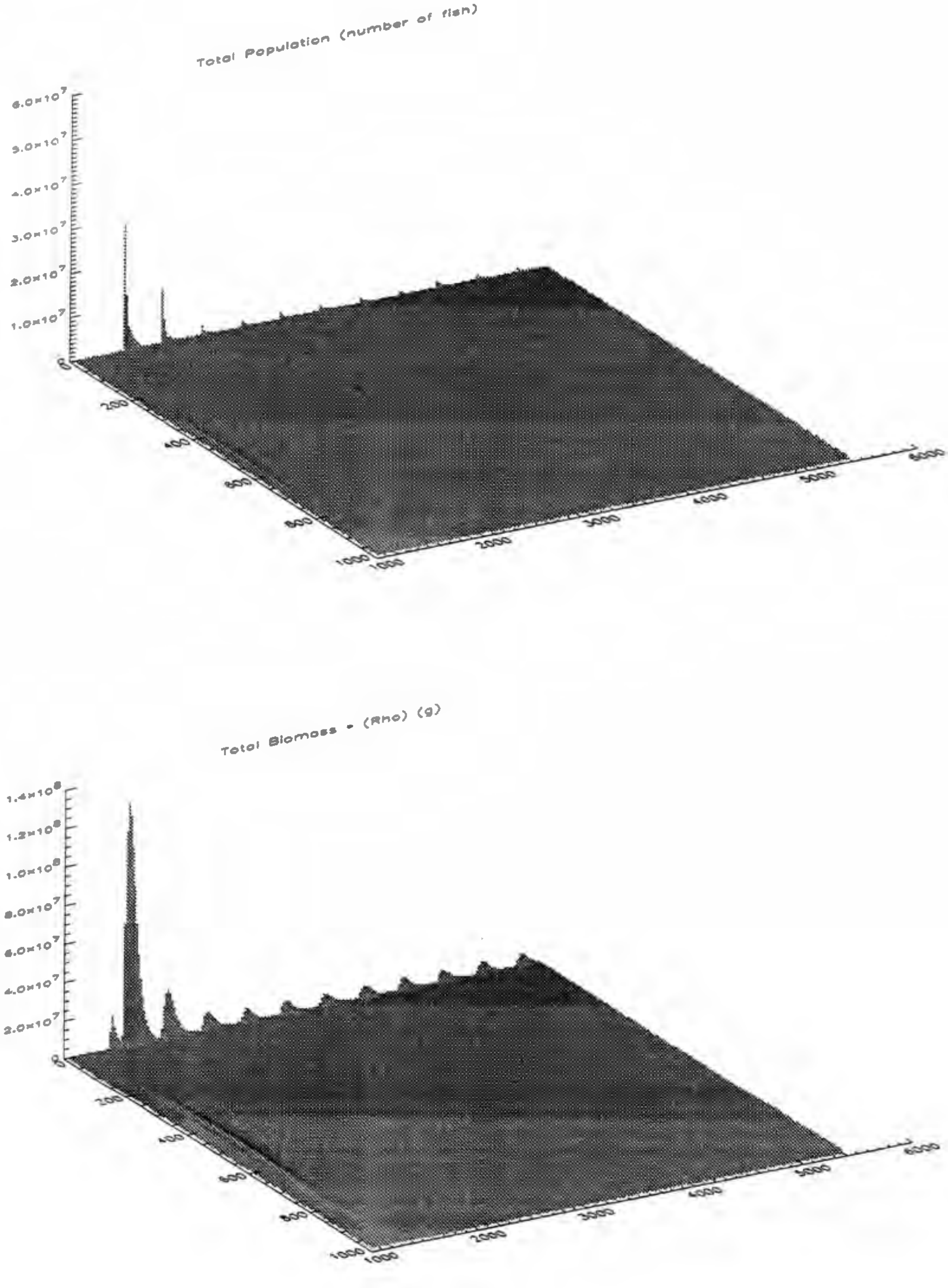


Figure 28: Total Fish Number and Biomass Distribution of *Case 5.1*

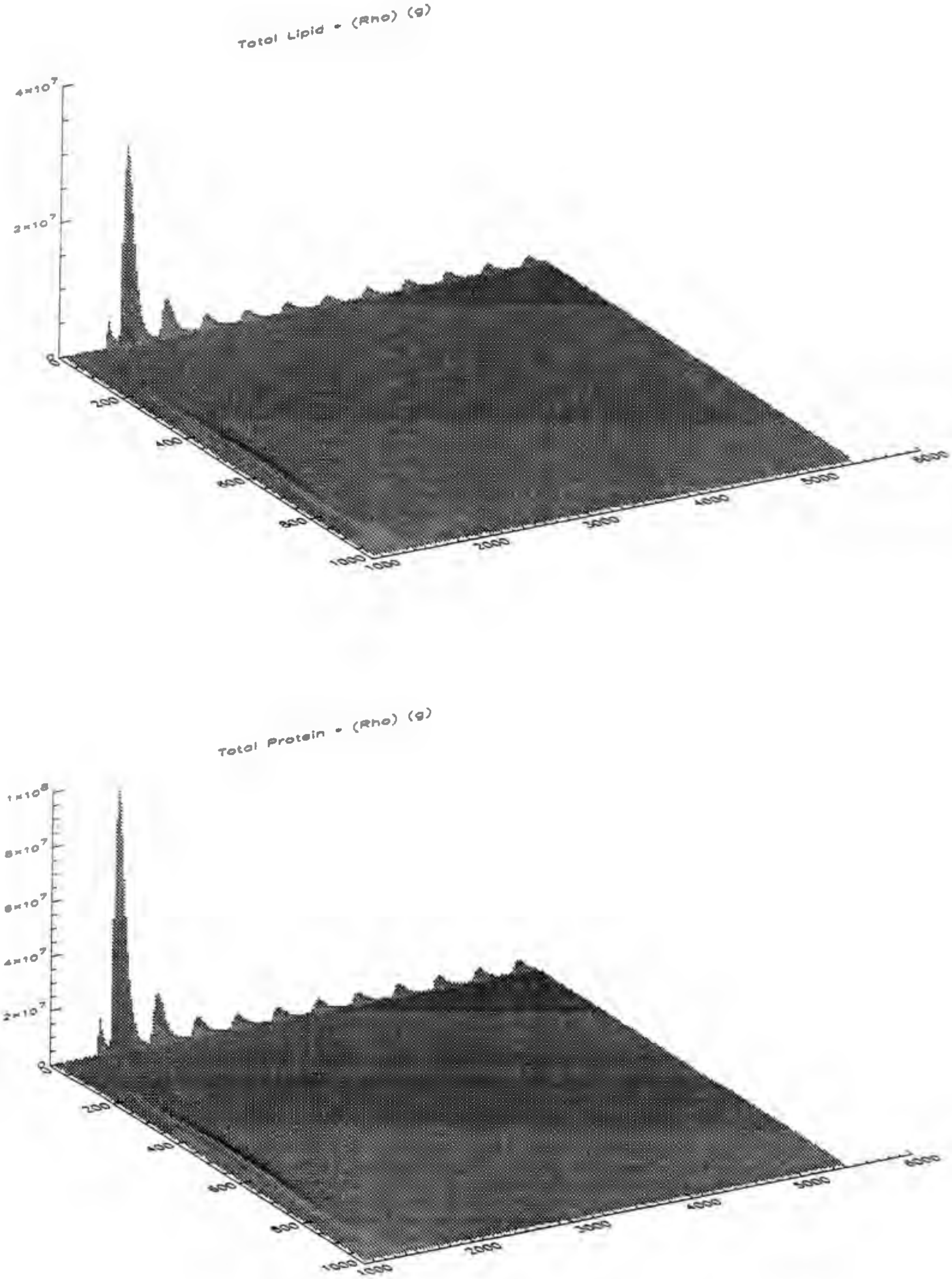


Figure 29: Total Lipid and Protein Distribution of *Case 5.1*

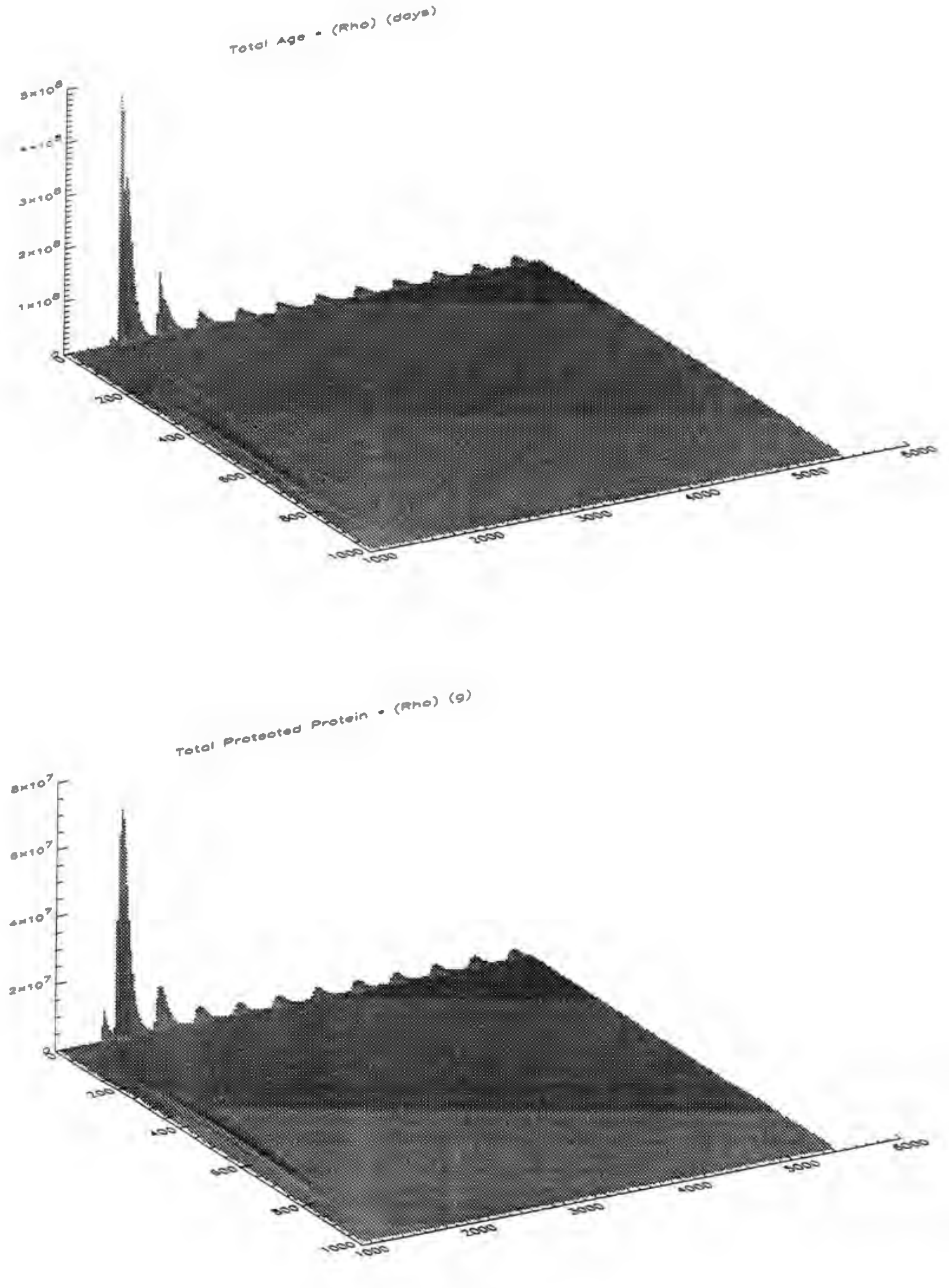


Figure 30: Total Age and Protected Protein Distribution of *Case 5.1*

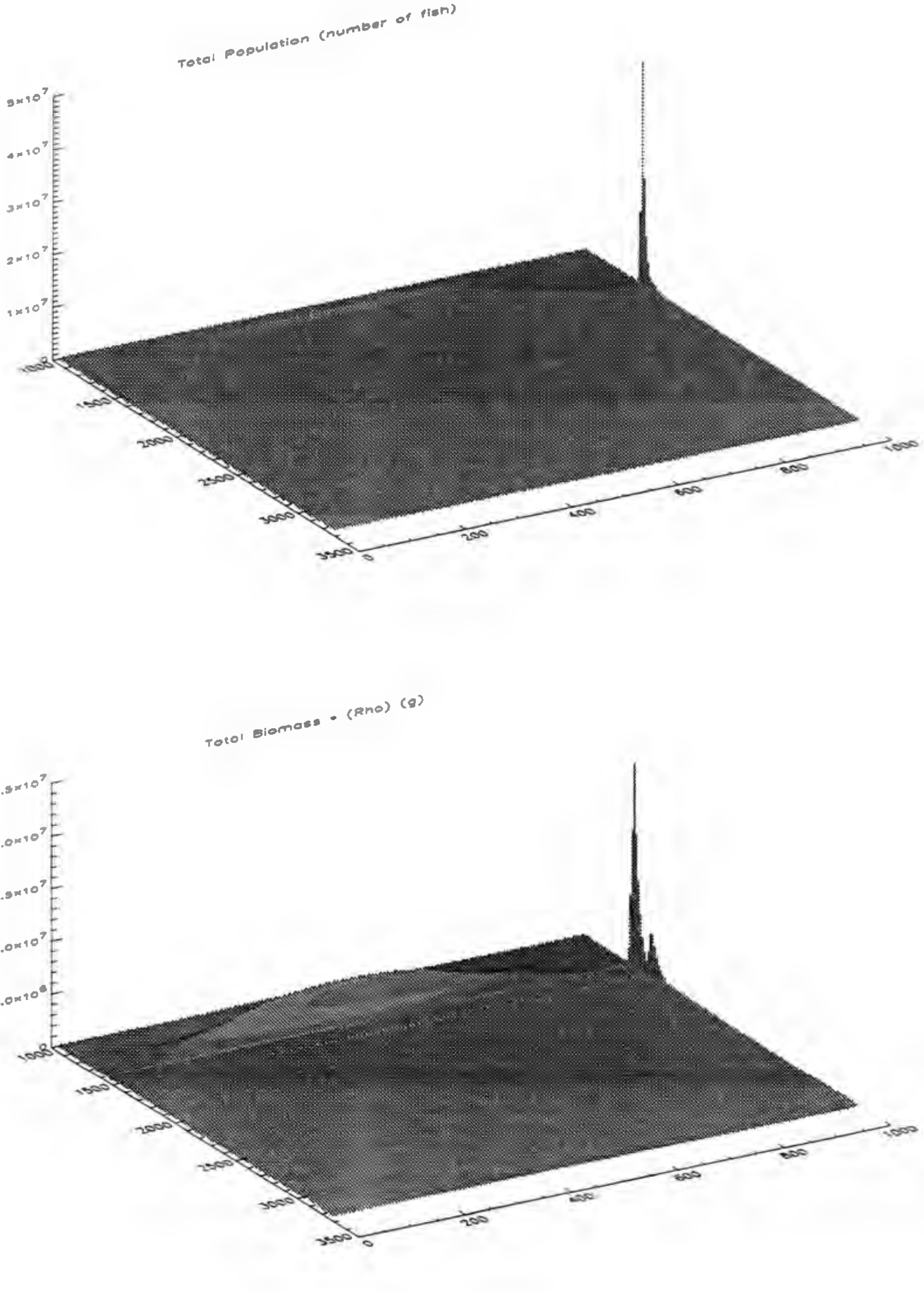


Figure 31: Total Fish Number and Biomass Distribution of *Case 5.2*

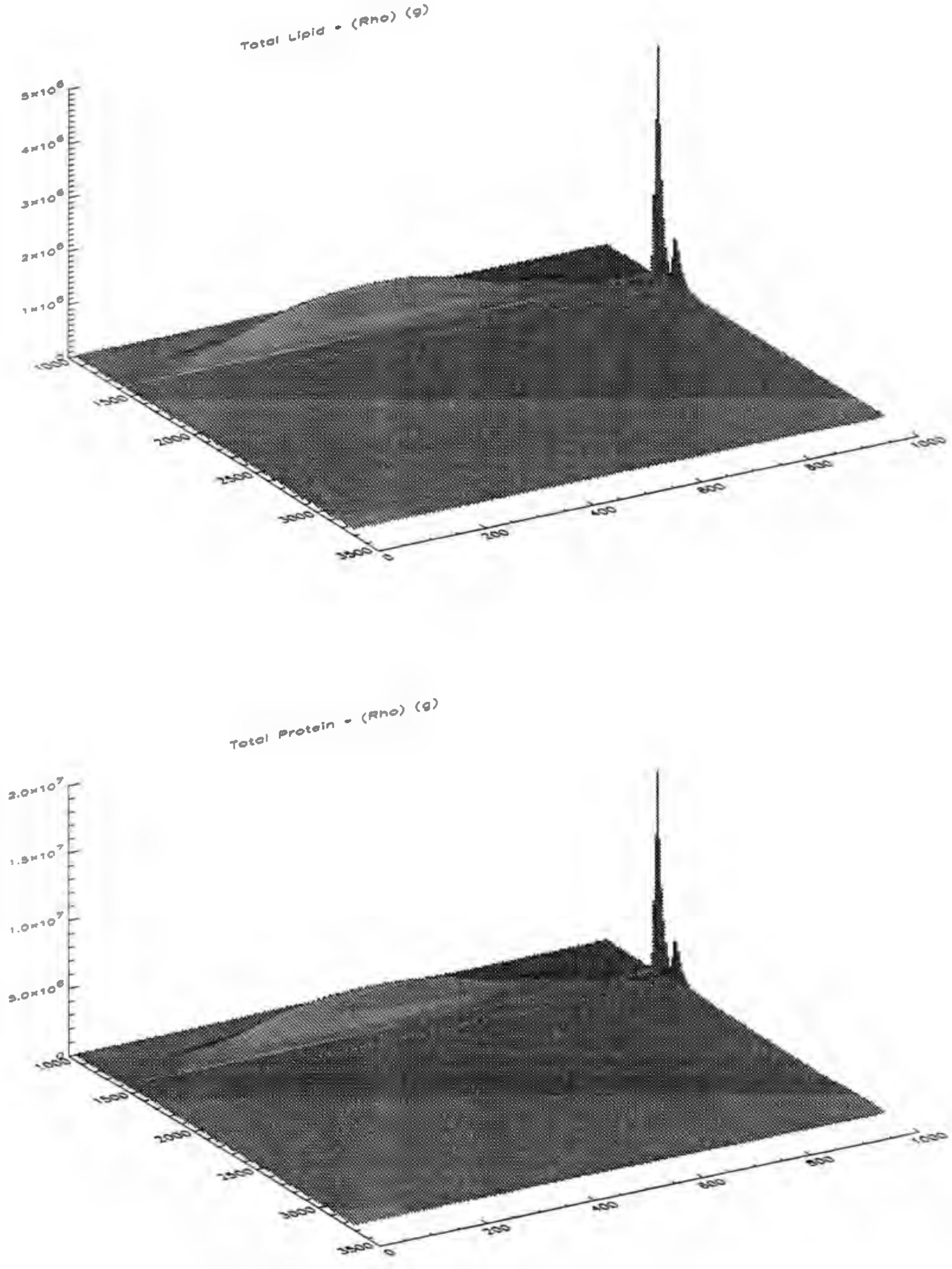


Figure 32: Total Lipid and Protein Distribution of *Case 5.2*

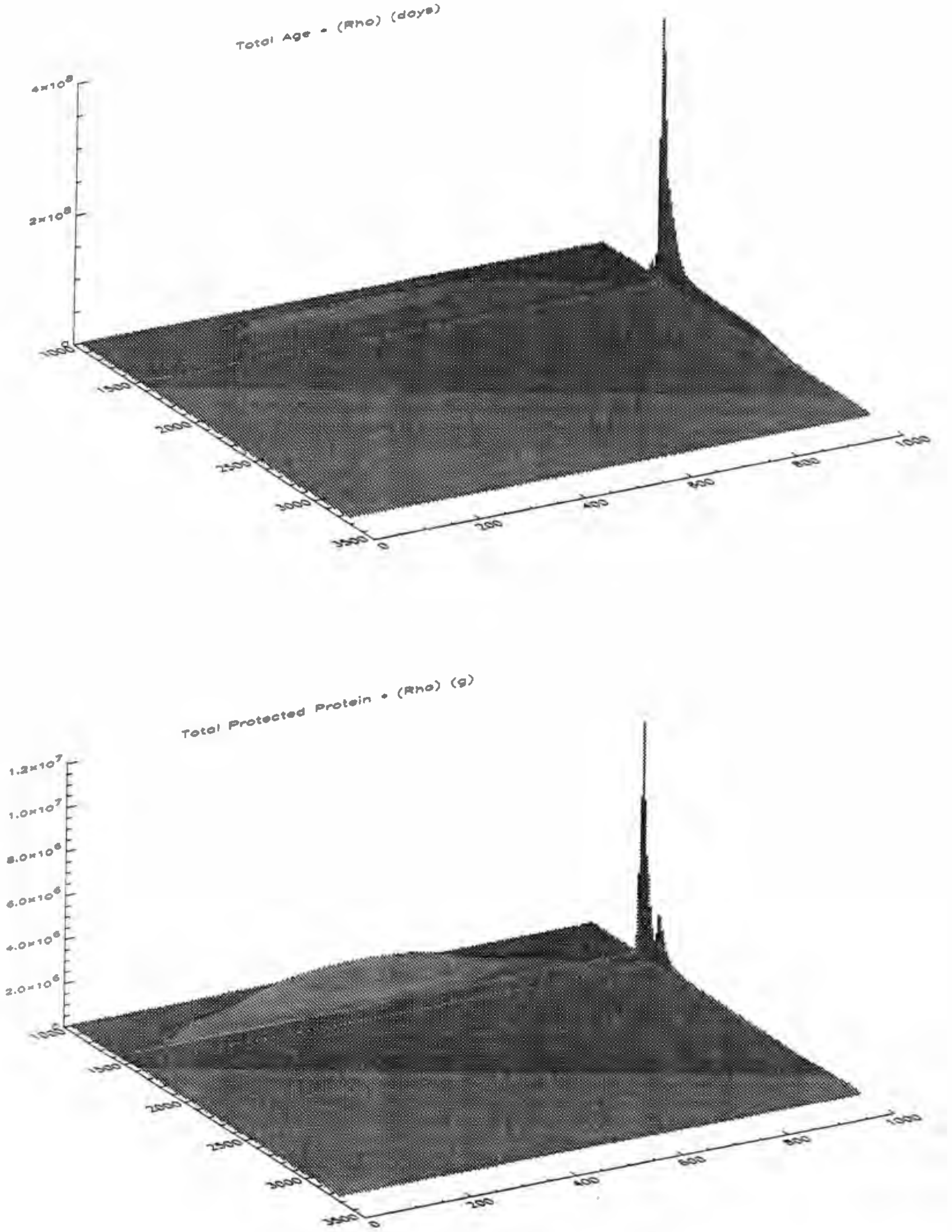
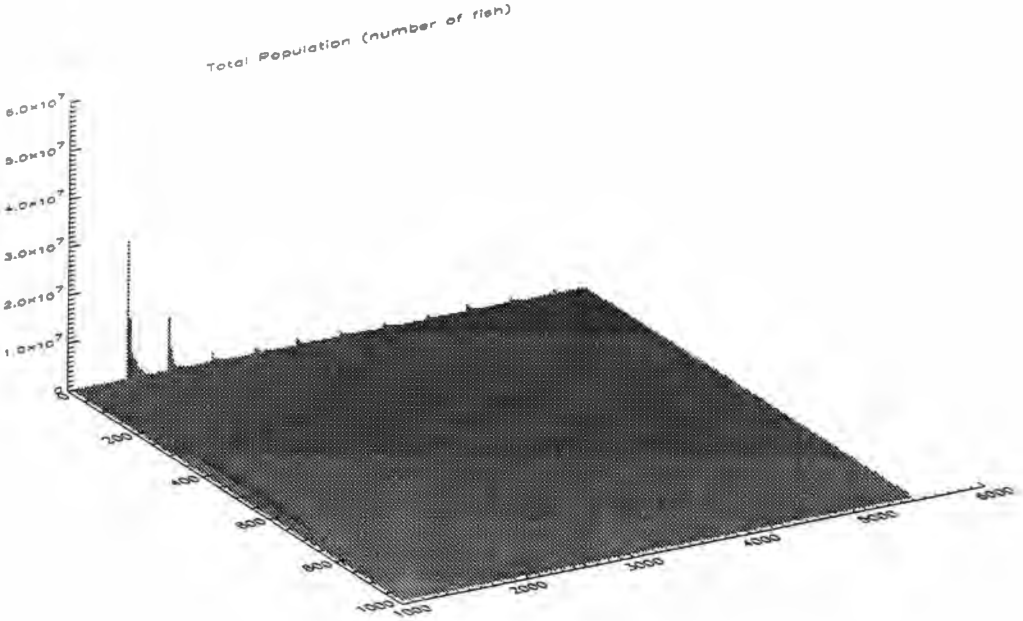


Figure 33: Total Age and Protected Protein Distribution of *Case 5.2*



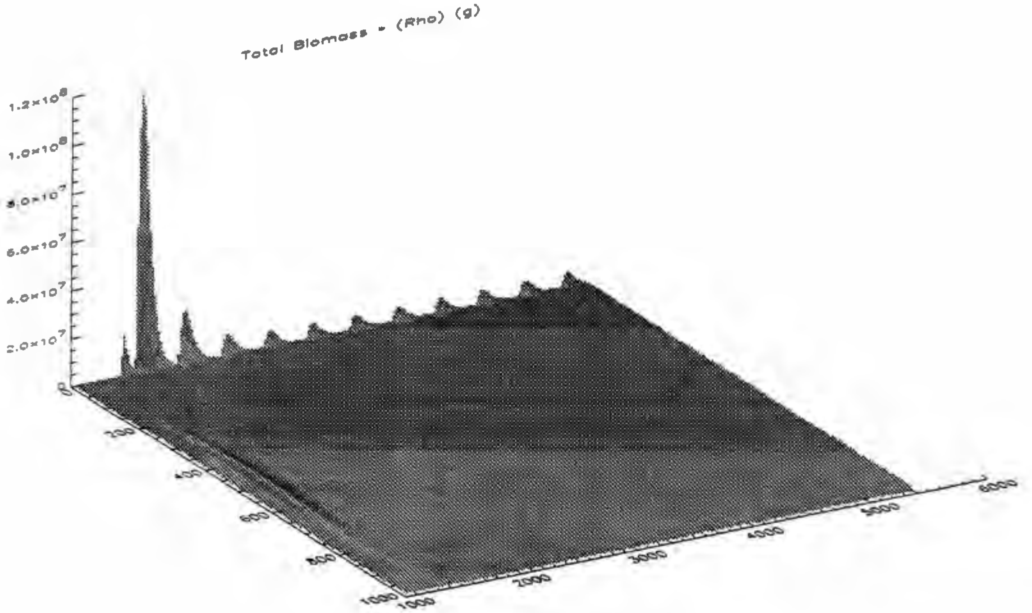


Figure 34: Total Fish Number and Biomass Distribution of *Case 5.3*

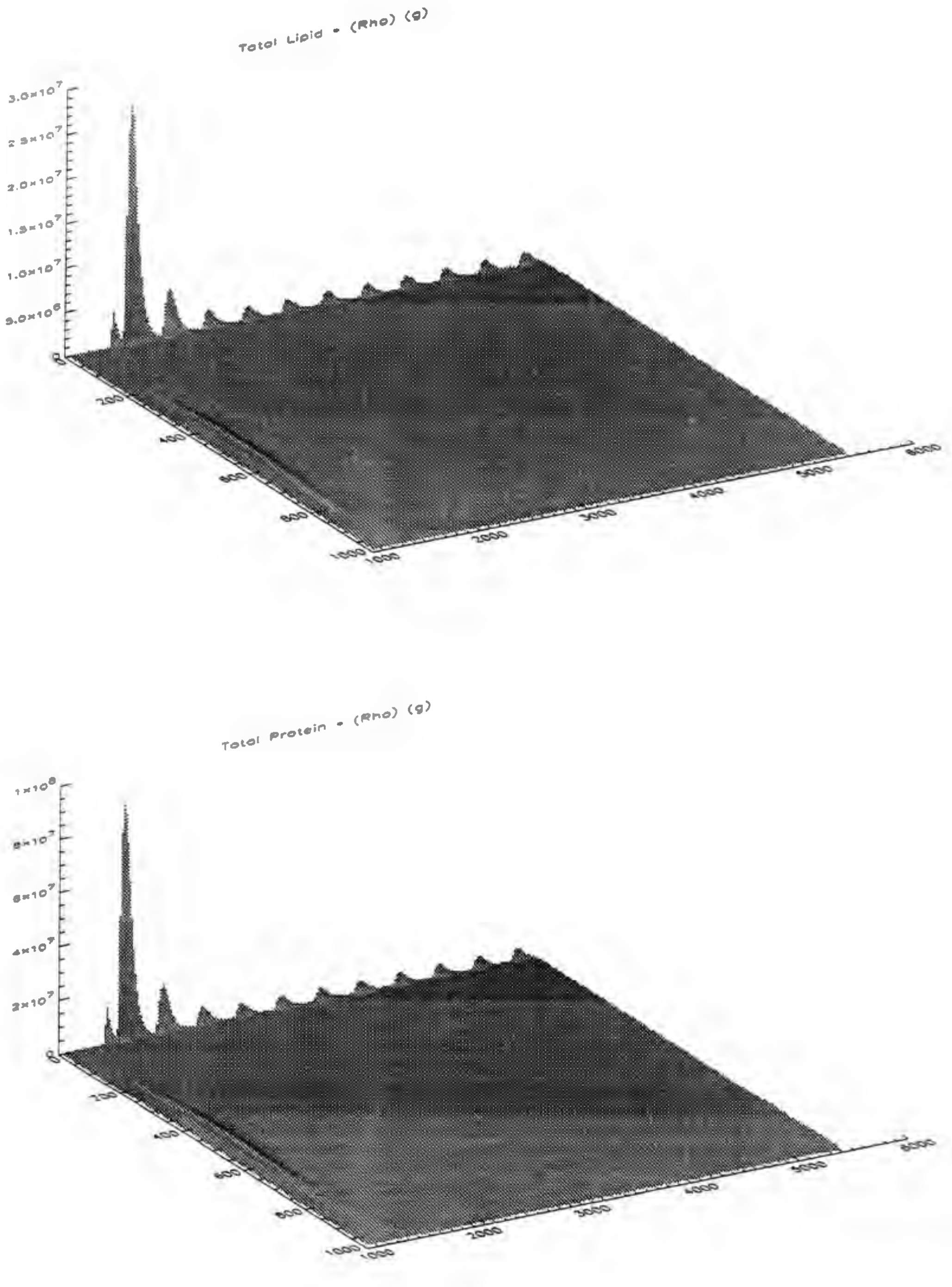


Figure 35: Total Lipid and Protein Distribution of *Case 5.3*

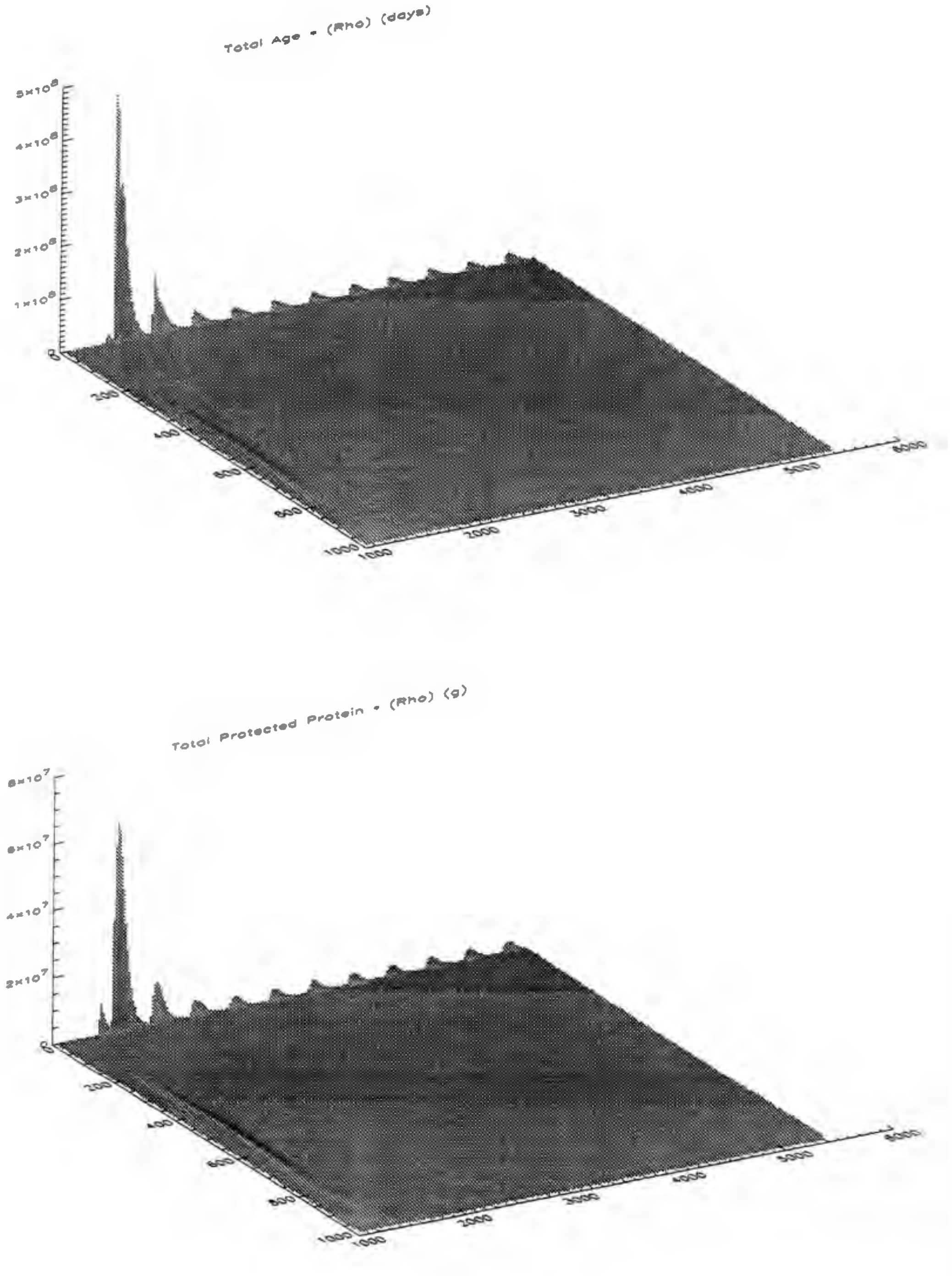


Figure 36: Total Age and Protected Protein Distribution of *Case 5.3*

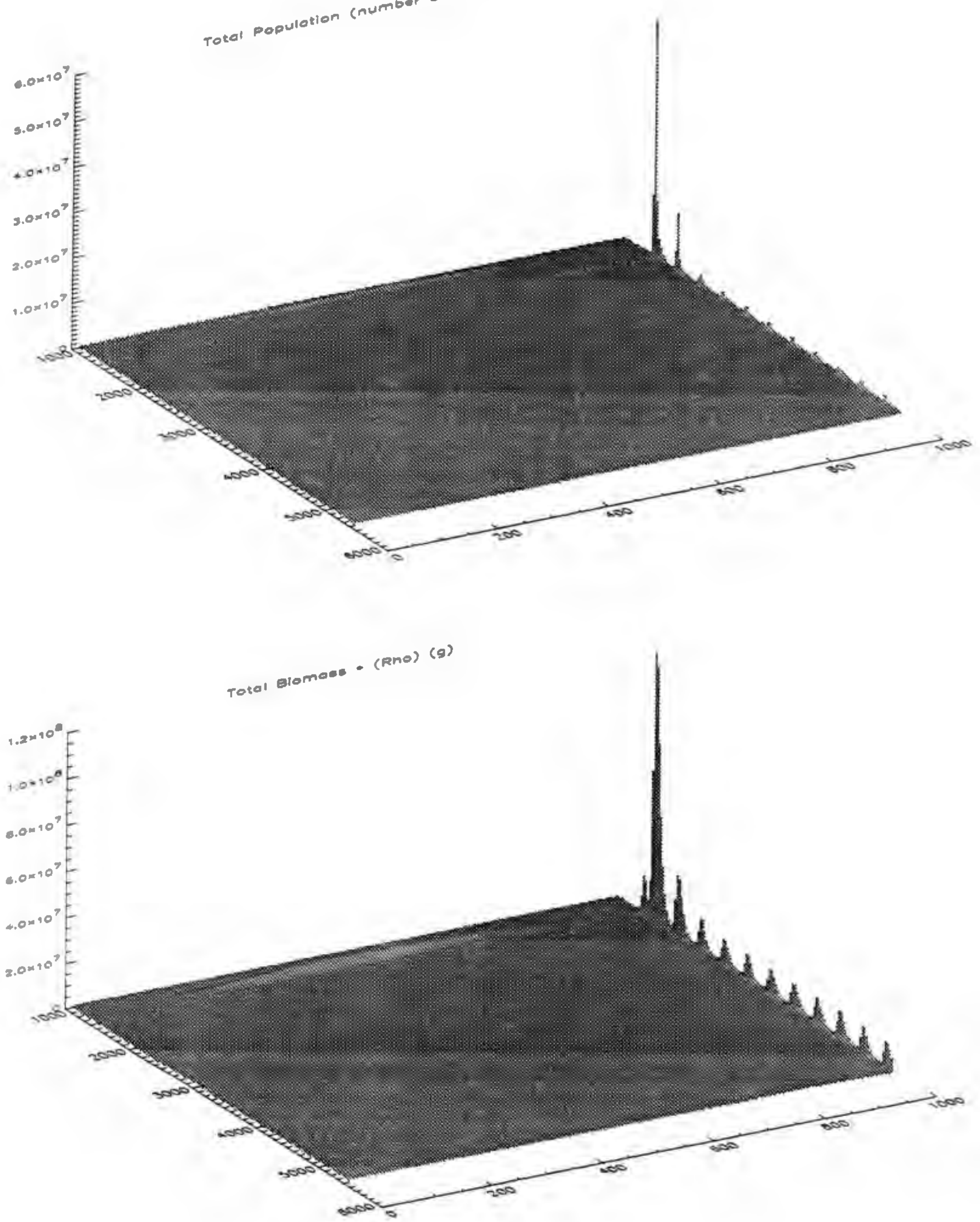


Figure 37: Total Fish Number and Biomass Distribution of *Case 5.4*

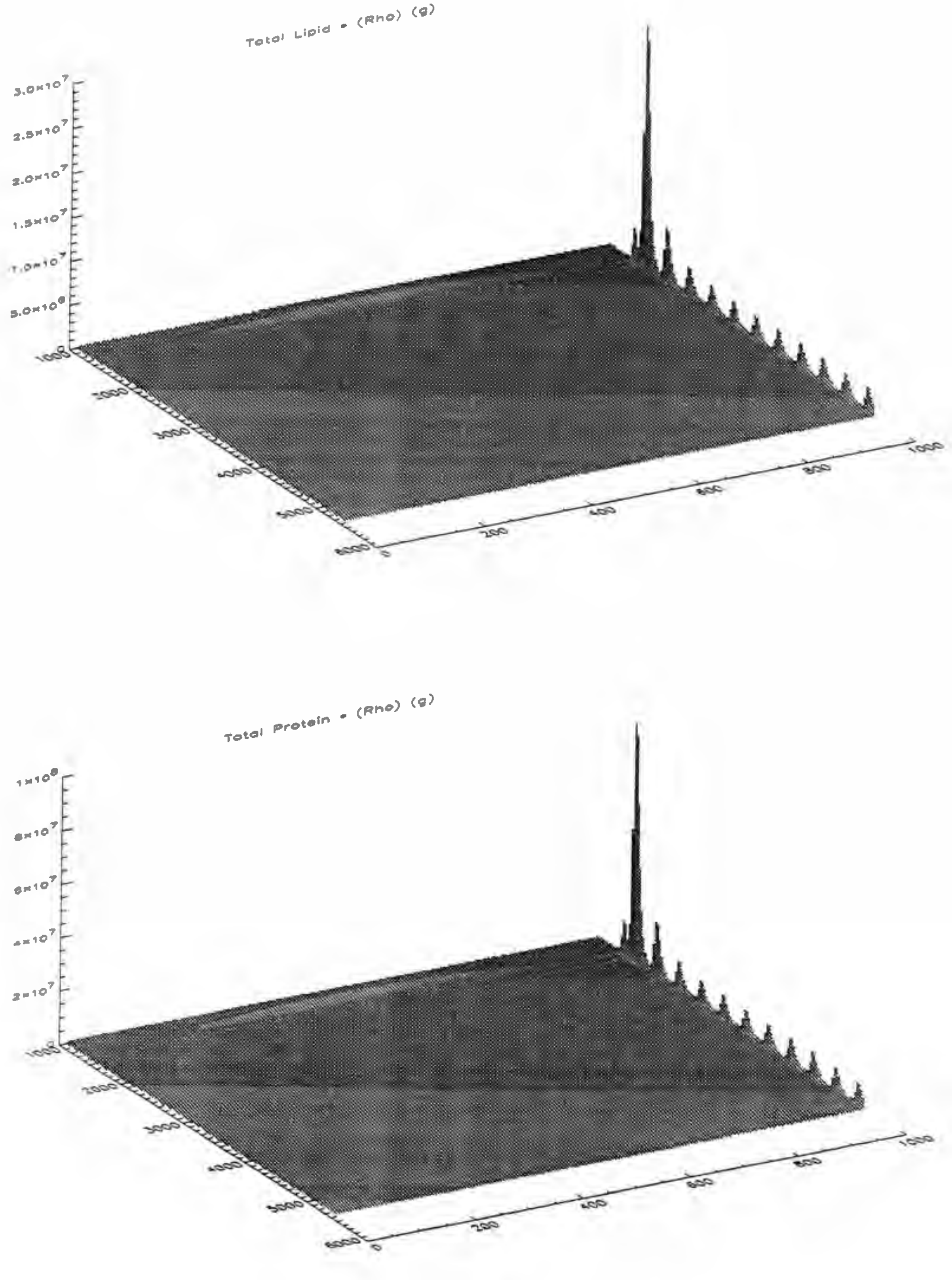


Figure 38: Total Lipid and Protein Distribution of *Case 5.4*

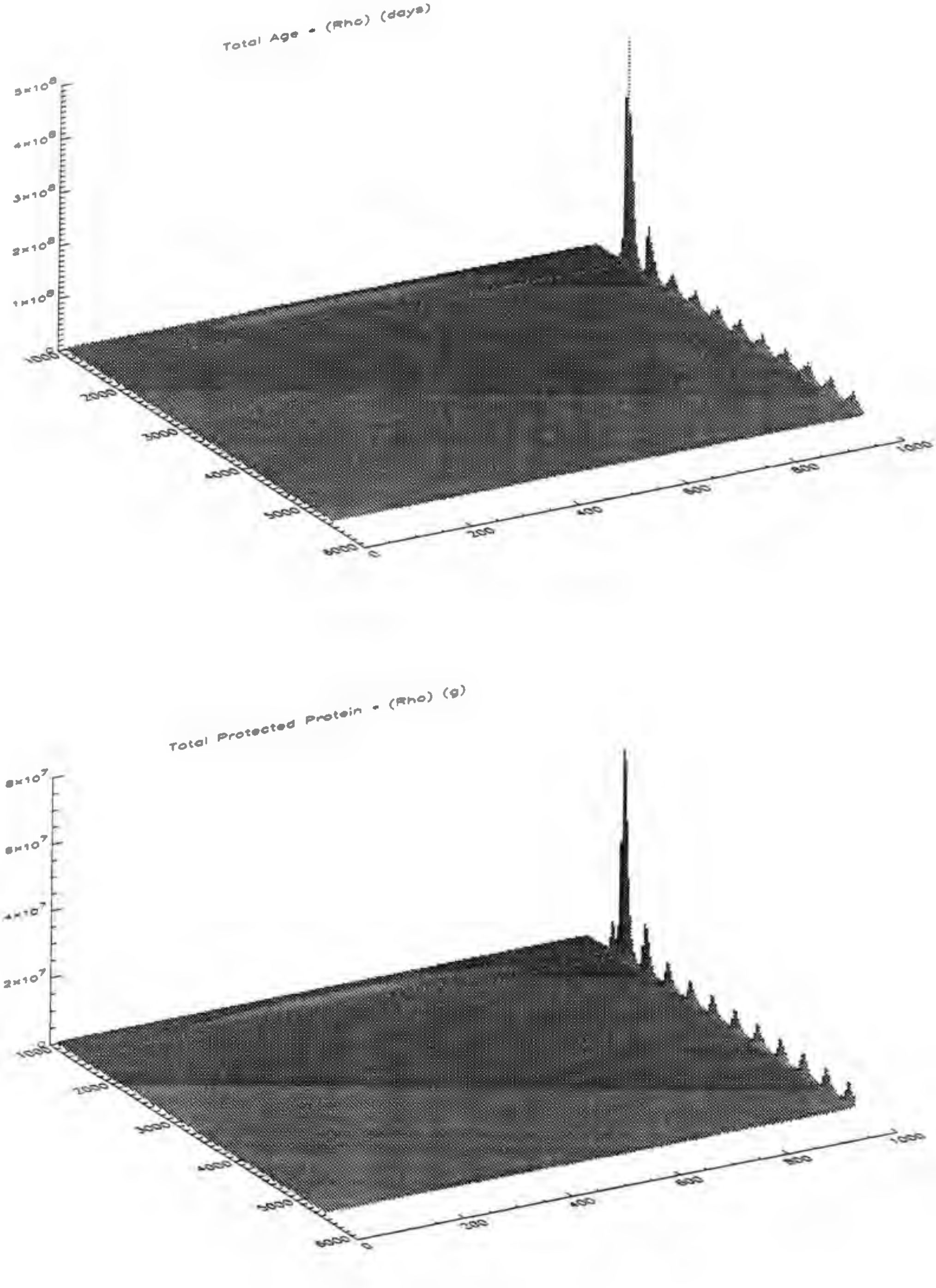


Figure 39: Total Age and Protected Protein Distribution of *Case 5.4*

Vita

Qingping Deng was born in Kunshang, Jiangsu Province, China, on October 4, 1963. He received his basic education in his home-town. He entered Soochow University, Suzhou, China, in September 1980. He received a Bachelor of Science degree in Mathematics in July of 1984 and a Master Science degree in Applied Mathematics in June of 1987 from Soochow University. Then he had worked as an instructor and research associate at the Institute of Computational Mathematics and Applied Software of Soochow University for more than five years. He enter the University of Tennessee, Knoxville, USA in 1993. He received a Master Science degree in Computer Science in October, 1997. He finished his Ph. D degree in Applied Mathematics (Mathematical Modeling & Computational Science) in December 1999.