

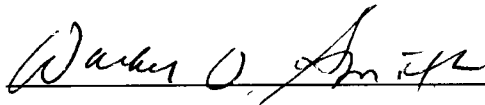
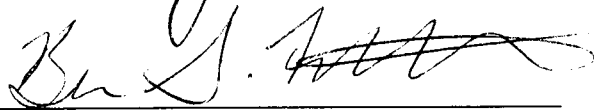
To the Graduate Council:

I am submitting herewith a dissertation written by Azmy Sima'an Ackleh entitled "Modeling Biological Processes in Aggregation of Phytoplankton." I have examined the final copy of this dissertation for form and content and recommend that it be accepted in partial fulfillment of the requirements for the degree of Doctor of Philosophy, with a major in Mathematics.



T. G. Hallam, Major Professor

We have read this dissertation
and recommend its acceptance:



Accepted for the Council:



Associate Vice Chancellor
and Dean of The Graduate School

**MODELING BIOLOGICAL PROCESSES IN
AGGREGATION OF PHYTOPLANKTON**

A Dissertation

Presented for the

Doctor of Philosophy

Degree

The University of Tennessee, Knoxville

Azmy Sima'an Ackleh

August 1993

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DEDICATION

This dissertation is dedicated to

my parents

Mr. Sima'an Elias Ackleh

سمعان الياس عاقله

and

Mrs. Wedad Toufique Ackleh

ولاد توفيق عاقله

who are my guiding light and inspiration.

My scholastic achievements would not have been possible

without their patience, encouragement, support and love.

Thanks Mom and Dad,

I love you.

شكراً يا ابي ويا اُمي الناس على قلبي
يا ابي ويا ابي

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ness, encouragement and support throughout my educational career; as well as my sister-in-law Hanan and my brother-in-law Riad for their kindness and encouragement.

ABSTRACT

The purpose of this study is to model the dynamics of phytoplankton by including the aggregation process. Aggregation, the formation of large particles from the collisions of smaller ones, is fundamental to many biological processes in the ocean. Because larger particles tend to sink faster than smaller ones, coagulation can be important in accelerating the export of organic matter from the ocean's surface to the deep sea and, consequently, it has the potential to limit phytoplankton populations on seasonal time scales.

A fundamental but unresolved problem associated with aggregation processes is the determination of the "stickiness function", a measure of the ability of particles to adhere to other particles. This leads to an inverse problem associated with a class of nonlinear integro-differential equations. In this dissertation we develop convergence theory for this algal coagulation model utilizing a spline-based collocation scheme within the context of the parameter identification problem.

Even though algal species are most directly affected by coagulation, the oceanographic food web is also impacted, at least indirectly, by the aggregation process. To better understand the role of the coagulation process in oceano-

graphic processes, in this dissertation we investigate the dynamics of a structured algal population in the context of a food chain model setting. While our efforts are generic in character, we focus specifically upon diatoms for parameterization. The food chain model incorporates nutrient dynamics as well as the dynamics of grazing. The algal species is modeled according to individual life history describing cell growth and the reproductive process.

The estimation of the "stickiness function" using the inverse method yielded remarkable results under ideal conditions (the observed data is identical to the model output). The model simulations demonstrate that the presence of grazers influence algal population dynamics by generating cyclic behavior of aggregate densities and changing the length of the bloom period. The number of living cells in aggregates is also fundamental to the food chain dynamics as increasing numbers of live cells can enhance coagulation.

TABLE OF CONTENTS

Part I.	INTRODUCTION	1
Part II.	APPROXIMATION AND PARAMETER ESTIMATION PROBLEM FOR ALGAL AGGREGATION MODELS	9
Part III.	THE ROLE OF AGGREGATE FORMATION IN PHYTOPLANKTON BLOOM DYNAMICS	45
Part IV.	WORK IN PROGRESS ON ESTIMATION OF PARAMETERS IN THE AGGREGATION PROCESS	91
Part V.	SUMMARY	110
	APPENDICES	115
	Appendix I	116
	Appendix II	125
	VITA	128

LIST OF TABLES

Part II.

Table 1	$\beta(x, y) = \beta^0$ with 10×10 data points.	28
Table 2	$\beta(x, y) = \beta^0 + \beta^1(x + y)$ with 10×10 data points.	29
Table 3	$\beta(x, y) = \beta^0$ with 10×10 data points and noise.	29
Table 4	$\beta(x, y) = \beta^0 + \beta^1(x + y)$ with 10×10 data points and noise.	29

Part III.

Table 1	Parameter values and units used in the model.	89
----------------	---	----

LIST OF FIGURES

Part II.

- Fig. 1.** The output of the collocation method using the approximation value β^{0^N} in the first row of Table 3. 30
- Fig. 2.** The observations generated by adding noise to the collocation method output using the standard deviation in row 1 of Table 3. 30
- Fig. 3.** The difference between the observations and the collocation method output. 31
- Fig. 4.** The graph of the density at size 1 (this size was picked arbitrarily from the sizes 1-10, similar results hold for the other sizes) versus time. 31
- Fig. 5.** The analogue of Fig. 1. but for the second form of β ($\beta(x, y) = \beta_0 + \beta_1(x + y)$) using the parameter values in row 1 of Table 4. 32
- Fig. 6.** The analogue of Fig. 2. but for the second form of β ($\beta(x, y) = \beta_0 + \beta_1(x + y)$) using the parameter values in row 1 of Table 4. 32
- Fig. 7.** The analogue of Fig. 3. but for the second form of β ($\beta(x, y) = \beta_0 + \beta_1(x + y)$) using the parameter values in row 1 of Table 4. 33
- Fig. 8.** The analogue of Fig. 4 but for the second form

of β ($\beta(x, y) = \beta_0 + \beta_1(x + y)$) using the
parameter values in row 1 of Table 4. 33

Part III

Fig. 1.	Conceptual representation of the biological interactions in the algal-grazer community.	67
Fig. 2.	The change of volume of a single cell with respect to time. The maintenance requirement b is set equal to A) $0.0084 d^{-1}$ B) $0.04 d^{-1}$ and C) $0.1 d^{-1}$.	68
Fig. 3.	The change of volume of a single cell with respect to time. The nutrient value N is equal to $25 \mu M$.	70
Fig. 4.	The probability $f(x)$ of a zooplankter ingesting an aggregate of size x when $x_{max} = 0.02 mm^3$.	71
Fig. 5.	The simulated response of the phytoplankton population dynamics.	72
Fig. 6.	The simulated response of the phytoplankton population development.	75
Fig. 7.	Long term oscillatory behavior of the phytoplankton population.	76
Fig. 8.	The effects of cell division on aggregates density.	78
Fig. 9.	The effect of nutrient concentration on the phytoplankton population.	79

Fig. 10.	The effect of the cell size on the phytoplankton dynamics.	81
Fig. 11.	The effects of the mixed layer depth on the phytoplankton dynamics.	83
Fig. 12.	The effects of the stickiness on aggregate formation.	85
Fig. 13.	The effects of inclusion of a carrying capacity on phytoplankton.	87

Part IV

Fig. 1.	The functional axis represents the density of the single cell algal population using the above three forms of s .	106
Fig. 2.	The functional axis represents: A) The output of the model using the stickiness function represented in Eq.(11). B) The observed data found by Riebesell (1991a). C) The difference between A) and B).	107

Appendix I

Fig. 1.	The functional axis represents: A) The exact solution of (1). B) The approximation solution of (1) using the collocation method. C) The difference between the exact and the approximation solutions of (1).	120
----------------	--	-----

Fig. 2.	The effect of finite interval length on the approximation.	122
Fig. 3.	The functional axis represents the approximation error.	124

Appendix II

Fig. 1	The functional axis represents the density of single cells using different values of zooplankton initial density ($0.5 \text{ \#}/L$, $0.05 \text{ \#}/L$).	125
Fig. 2.	The functional axis represents the density of zooplankton using different values of zooplankton initial density ($0.5 \text{ \#}/L$, $0.05 \text{ \#}/L$).	126
Fig. 3.	The functional axis represents the density of aggregates using the value $0.5 \text{ \#}/L$ for zooplankton initial density.	126
Fig. 4.	The functional axis represents the density of aggregates using the value $0.05 \text{ \#}/L$ for zooplankton initial density.	127

Part I

INTRODUCTION

Seasonally high nutrient concentrations in regions of the oceans often result in algal blooms with the consequent high biomass and particle concentration. A bloom usually ends when the algae deplete their nutrient supply, slow their growth, and sink out of surface waters or are consumed by zooplankton. During a bloom, coagulation can be an important factor controlling the fate of algal populations. Coagulation is the process by which small particles are converted into larger, faster settling particles. When two particles collide there is a chance they will stick together to form a larger particle. Multiple collisions can produce relatively large aggregates; for example, aggregates greater than 1mm are produced from particles less than $10\mu\text{m}$ (Jackson and Lochmann, 1992).

Oceanic aggregates are composed of a variety of biologically derived organic materials, including algal cells, fecal pellets, and animal feeding structures, such as mucus nets from pteropods and larvacean feeding structures (Alldredge and Silver, 1988). Marine aggregates have been observed to increase in size with increasing depth (Kranck and Milligan 1990). A number of models have suggested that aggregate formation is a quantitatively significant loss process (Jackson 1990; Hill 1992), and recent studies in the North Sea reinforce the suggestion that coagulation is an important process for determining the fate of organic matter produced by phytoplankton blooms (Riebesell 1991 a,b).

Inherent to the aggregation process is the concept of "stickiness" : when two particles collide, there is some chance they will stick together to form larger particles. Laboratory studies (Kiorboe et al., 1990) and field experiments (Alldredge et al. 1993, preliminary report) have shown that algal cells have a positive probability to coagulate when they collide. However, the principal factors governing stickiness remain unclear. One hypothesis is that algal stickiness is a function of available nutrients. Kiorboe et al., (1990) showed that stickiness increases when nutrients are depleted from the medium. However, recent experiments have suggested that there is only a weak relationship between nutrient concentration of the medium and the probability of one cell's sticking to another (Alldredge et al. 1993, preliminary report).

To improve our understanding of the aggregation process, we have initiated a study to determine the role of biological processes in coagulation. Part II of this dissertation examines theoretical and numerical aspects of an integro-differential equation model of coagulation of algae into aggregates. We begin with the following differential equation:

$$\begin{cases} \frac{\partial \rho(t, x)}{\partial t} = \frac{1}{2} \int_0^x \beta(x-y, y) \rho(t, x-y) \rho(t, y) dy - \rho(t, x) \int_0^A \beta(x, y) \rho(t, y) dy \\ \rho(0, x) = \rho_0(x). \end{cases} \quad (1)$$

The x variable represents the size (mm^3) of the aggregate, and the t variable represents time. The function $\rho(t, x)$ is the density of aggregates of size x at time

t and the “stickiness function” $\beta(x, y)$ represents the probability of an aggregate of size x sticking to an aggregate of size y . The first term in the above equation expresses the rate at which collisions occur to form new particles with the size x to $x + dx$ while the second term expresses the rate at which collisions cause particles to be lost from the same interval.

Equations of the type (1) arise in various applications involving particle aggregation (Smoluchowski, 1917; Gelbard and Seinfeld, 1978; Jackson, 1990; Jackson and Lochmann 1992). Smoluchowski (1917) used this equation to investigate the kinetics of the coagulation of colloidal solutions. In Gelbard and Seinfeld’s paper (1978) this equation is used to describe the state of a spatially and chemically homogeneous particulate system. In the dynamics of such a system, individual particles may grow through accretion of material from the fluid phase or they may shrink by loss of material. In addition to changing size by the biological processes involved in growth, particles may collide and, subsequently, they may coagulate. Jackson (1990) and Jackson and Lochmann (1992) have used equation (1) to describe the effect of coagulation on algal blooms.

To apply this model as a predictive tool, we must be able to compute solutions, and we must know the stickiness function. Spline-based collocation methods were originally proposed for equations of form (1) in Gelbard and Seinfeld (1978) in a semi-discrete formulation:

$$\begin{aligned}\frac{\partial \rho^N(t, x)}{\partial t} &= \pi^N \frac{1}{2} \int_0^x \beta(x-y, y) \rho^N(t, x-y) \rho^N(t, y) dy \\ &- \pi^N \rho^N(t, x) \int_0^A \beta(x, y) \rho^N(t, y) dy,\end{aligned}$$

where

$$\rho^N(t, x) = \sum_{k=1}^N \alpha_k^N(t) B_k^N(x)$$

denotes the computational approximation. Here B_k^N denotes either a linear spline or cubic B-spline basis function, and π^N is the corresponding interpolation operator. Collocation leads to a nonlinear system of ordinary differential equations for the coefficients α_k^N by evaluation at the collocation grid points. The choice of collocation, as opposed to the Galerkin approximation, is advantageous because of the simplicity of implementation (Gelbard and Seinfeld, 1978).

A problem in implementing this numerical technique to predict algal aggregation behavior is that the stickiness function is not available directly from laboratory experiments. In fact, the quantities that have been obtained in experimental settings are values of the size densities (Riebesell, 1991a,b). Estimates of stickiness have been attempted recently but the approaches have led to biologically unrealistic stickiness functions in many cases. To estimate the stickiness function, we consider a least squares formulation and seek to minimize

$$J(\beta) = \sum_{i,j} |\rho(t_i, x_j; \beta) - z_{i,j}|^2$$

where $\{z_{i,j}\}$ denotes the observed size-density data and $\rho(t, x; \beta)$ denotes the dependence of the solution of (1) on the parameter β .

The models of Jackson (1990), Hill (1992) and Jackson and Lochmann (1992) focused primarily on the role of physical processes in the coagulation of phytoplankton. These models parameterized algal growth as being either constant (Jackson 1990) or nutrient and irradiance dependent (Jackson and Lochmann, 1992). The conclusions from these models were that coagulation can limit phytoplankton yields and accelerate the removal of senescent cells by aggregating them into larger, more rapidly sinking particles. Hill (1992) suggested that only in regions which attain high densities of phytoplankton can random collision occur frequently enough to produce significant aggregate formation and high rates of vertical flux. Although these models revealed the importance of coagulation in limiting phytoplankton population size, they have not included detailed biological description of the phytoplankton or the role of resource-consumer interactions.

Part III of this dissertation focuses on algal population dynamics and presents a food-chain model in which the effects of biological processes at the individual level are incorporated. Growth of phytoplankton cells is modeled as a function of cell volume, and the dynamics of phytoplankton, zooplankton, and nutrients are represented in a simple resource-consumer model. Understanding the interactions between food chain dynamics and coagulation can clarify the role of the coagulation in limiting phytoplankton populations. Aggregation should be especially important ecologically in regimes with high nutrients and low zooplankton densities (Jackson and Lochmann, 1992). The subsequent development concentrates on the phytoplankton trophic level by including detailed representations of the

biological aspects of the algal population and employing generic, nonstructured descriptions for nutrient and grazer dynamics. The lack of structure in the zooplankton community is an initial approximation, but this level of resolution allows inference of the importance of grazing.

This dissertation consists of 5 parts. The outline of Part II is as follows. Collocation approximations and their convergence are the subjects of Section 2. In Section 3 we study convergence issues associated with the inverse problem. Section 4 contains some numerical examples to illustrate the techniques analyzed here. In Section 5, we give some remarks on more sophisticated, biologically relevant models and future research issues. For completeness, we discuss existence, uniqueness, and regularity issues of (1) in the Appendix.

Part III is structured by beginning with the description of the food chain model in Section 2. Section 3 contains the results of our simulations. In Section 4 we present the conclusions that delineate the roles of aggregation in the oceans. The numerical methodology used for obtaining the simulations in this paper is given in the Appendix.

In Part IV we modify the model discussed in Part III to include self-shading effects and use inverse methodology to get an initial estimate on the "stickiness parameter" for the observed data of Riebesell (1991a,b). In Part V we give some concluding remarks and some future research issues. In Appendix I we discuss the numerical procedure and the approximation error due to this method while in Appendix II the effect of initial zooplankton density on the phytoplankton bloom

period is covered.

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Part II

APPROXIMATION AND PARAMETER ESTIMATION PROBLEMS FOR ALGAL AGGREGATION MODELS*

Abstract - Aggregation processes are intrinsic to many biological phenomena including sedimentation and coagulation of algae during bloom periods. A fundamental but unresolved problem associated with aggregate processes is the determination of the "stickiness function", a measure of the ability of particles to adhere to other particles. This leads to an inverse problem associated with a class of nonlinear integro-differential equations. The purpose of this article is to develop convergence theory for this algal coagulation model utilizing a spline-based collocation scheme within the context of the parameter identification problem.

1. Introduction

Coagulation, the formation of large particles from multiple collisions of smaller ones, is fundamental to many biological processes in the ocean including algal population dynamics. The aggregation of oceanic particles has the potential to limit phytoplankton populations and it is possible that the aggregation process

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could be as important as grazing in the ocean. Grazing has been widely studied but the investigation of coagulation in oceanographic processes is still in its infancy.

Aggregates in the ocean seldom consist of algal cells alone but are rather composites of algae with inorganic and other organic matter. Fundamental to coagulation is the "stickiness" characteristics of the aggregative system. When two particles collide, there is a chance they will stick together to form larger particles. Stickiness is responsible for the creation of particles several orders of magnitude larger than the size of single cells. For example, Jackson and Lochmann (1992) have indicated that multiple collisions can produce particles exceeding 1 mm from particles of size $10\mu m$. Algal cells are subjected to the same physical forces as other oceanic particles and because there is a finite chance that upon collision they also will stick, algal cells can coagulate to form large flocs (Kiorboe et al., 1990; Riebesell 1991). Aggregate formation and the vertical fluxes associated with increased particle mass have been observed to be important processes in the removal of particles from ocean's surface to the deep sea. The coagulation of particles appears to be a fundamental biological process that could be important when determining global patterns of oceanographic carbon flux.

To improve our understanding of the aggregation process, we have initiated a study to determine the role of biological processes in coagulation. This article examines theoretical and numerical aspects of an integro-differential equation model of coagulation of algae into aggregates. We begin with the following differential equation:

$$\left\{ \begin{array}{l} \frac{\partial \rho(t, x)}{\partial t} = \frac{1}{2} \int_0^x \beta(x-y, y) \rho(t, x-y) \rho(t, y) dy - \rho(t, x) \int_0^A \beta(x, y) \rho(t, y) dy \\ \rho(0, x) = \rho_0(x). \end{array} \right. \quad (1.1)$$

The x variable represents the size (mm^3) of the aggregate, and the t variable represents time. The function $\rho(t, x)$ is the density of aggregates of size x at time t and the “stickiness function” $\beta(x, y)$ represents the probability of an aggregate of size x sticking to an aggregate of size y . The first term in the above equation expresses the rate at which collisions occur to form new particles with the size x and $x + dx$ while the second term expresses the rate at which collisions cause particles to be lost from the same interval.

Equations of the type (1.1) arise in various applications involving particle aggregation (Smoluchowski, 1917; Gelbard and Seinfeld, 1978; Jackson 1990; Jackson and Lochmann, 1992). Smoluchowski (1917) used this equation to investigate the kinetics of the coagulation of colloidal solutions. In Gelbard and Seinfeld’s paper (1978) this equation is used to describe the state of a spatially and chemically homogeneous particulate system. In the dynamics of such a system, individual particles may grow through accretion of material from the fluid phase or they may shrink by loss of material. In addition to changing size by the biological processes involved in growth, particles may collide and, subsequently, they may coagulate. Jackson (1990) and Jackson and Lochmann (1992) have used equation (1.1) to describe the effect of coagulation on algal blooms.

To apply this model as a predictive tool, we must be able to compute solutions, and we must know the stickiness function. Spline-based collocation methods were originally proposed for equations of form (1.1) in Gelbard and Seinfeld (1978) in a semi-discrete formulation:

$$\begin{aligned} \frac{\partial \rho^N(t, x)}{\partial t} &= \pi^N \frac{1}{2} \int_0^x \beta(x-y, y) \rho^N(t, x-y) \rho^N(t, y) dy \\ &\quad - \pi^N \rho^N(t, x) \int_0^A \beta(x, y) \rho^N(t, y) dy, \end{aligned}$$

where

$$\rho^N(t, x) = \sum_{k=1}^N \alpha_k^N(t) B_k^N(x)$$

denotes the computational approximation. Here B_k^N denotes either a linear spline or cubic B-spline basis function, and π^N is the corresponding interpolation operator. Collocation leads to a nonlinear system of ordinary differential equations for the coefficients α_k^N by evaluation at the collocation grid points. The choice of collocation, as opposed to the Galerkin approximation, is advantageous because of the simplicity of implementation (Gelbard and Seinfeld, 1978)

A problem in implementing this numerical technique to predict algal aggregation behavior is that the stickiness function is not available directly from laboratory experiments. In fact, the quantities that have been obtained in experimental settings are values of the size densities (Alldredge and Gotschalk, 1988; Riebesell, 1991). Estimates of stickiness have been attempted recently but the approaches have led to biologically unrealistic stickiness functions in many cases. To estimate the stickiness function, we consider a least squares formulation and seek to

minimize

$$J(\beta) = \sum_{i,j} |\rho(t_i, x_j; \beta) - z_{i,j}|^2$$

where $\{z_{i,j}\}$ denotes the observed size-density data and $\rho(t, x; \beta)$ denotes the dependence of the solution of (1.1) on the parameter β .

Our specific goals in this paper are to formally analyze convergence for the collocation methods and to examine computational issues related to the least squares approach to identifying the stickiness function β from observed size densities. The paper is organized as follows. Collocation approximations and their convergence are the subjects of Section 2. In Section 3 we study convergence issues associated with the inverse problem. Section 4 contains some numerical examples to illustrate the techniques analyzed here. In Section 5, we give some remarks on more sophisticated, biologically relevant models and future research issues. For completeness, we discuss existence, uniqueness, and regularity issues of (1.1) in the Appendix.

2. Convergence Analysis for Collocation Schemes

We begin this section by rewriting the differential equation in an operator form.

Define the nonlinear operator F by

$$F(\phi)(x) = \frac{1}{2} \int_0^x \beta(x-y, y) \phi(x-y) \phi(y) dy - \phi(x) \int_0^A \beta(x, y) \phi(y) dy,$$

which allows rewriting the differential equation (1.1) in the abstract form

$$\dot{\rho} = F(\rho),$$

where “ $\dot{}$ ” denotes time differentiation. For the state space, we consider two possibilities, $C[0, A]$ and $C^1[0, A]$, equipped with the usual norms, denoted by $\|\cdot\|_0$ and $\|\cdot\|_1$, respectively. As may be seen in the Appendix, it is a straightforward but tedious matter to establish the following existence and uniqueness results.

Theorem A.2. Suppose that $\rho_0 \in C[0, A]$, and that $\beta \in C([0, A] \times [0, A])$. Then, there exists a $T_0 > 0$ and a unique function $\rho \in C^1([0, T_0]; C[0, A])$ satisfying $\rho(0) = \rho_0$ and Eq. (1.1) on $[0, T_0]$.

Theorem A.3. Suppose that $\rho_0 \in C^1[0, A]$, and that $\beta \in C^1([0, A] \times [0, A])$. Then, there exists a $T_1 > 0$ and a unique function $\rho \in C^1([0, T_1]; C^1[0, A])$ satisfying $\rho(0) = \rho_0$ and Eq. (1.1) on $[0, T_1]$.

Theorem A.4. Suppose that $\rho_0 \in C[0, A]$ satisfies $\rho_0(x) \geq 0 \forall x \in [0, A]$ and $\rho_0(x) = 0$ for $x < x_{min}$, where $x_{min} \in [0, A]$ is a positive constant, and that $\beta \in C([0, A] \times [0, A])$ satisfies $\beta(x, y) = \beta(y, x)$ and $\beta(x, y) = 0$ if $(x + y) > A$. Then, there exists a unique function $\rho \in C^1([0, \infty); C[0, A])$ satisfying the following: $\rho(t, x) \geq 0 \forall x \in [0, A]$ and $\forall t \in [0, \infty)$ $\frac{d}{dt} \int_0^A x \rho(t, x) dx = 0$ and ρ is a global solution of (1.1).

Similarly, there exist a unique global solution $\rho \in C^1([0, \infty); C^1[0, A])$ if $\rho_0 \in C^1[0, A]$, $\beta \in C^1([0, A] \times [0, A])$ and they both satisfy the same conditions as in

Theorem A.4.

In the process of obtaining these results, some important inequalities arise that indicate how F and ρ depend on the stickiness function β . In particular, we have that

$$\|F(\phi) - F(\rho)\|_0 \leq L\|\phi - \rho\|_0 \text{ where, } L = \frac{3A}{2}\|\beta\|_0(\|\phi\|_0 + \|\rho\|_0) \quad (2.1)$$

$$\|F(\phi; \beta) - F(\phi; \hat{\beta})\|_0 \leq \frac{3A}{2}\|\beta - \hat{\beta}\|_0\|\phi\|_0^2 \quad (2.2)$$

$$\|F(\phi) - F(\rho)\|_1 \leq L_1\|\phi - \rho\|_1 \text{ where, } L_1 = \frac{9A+1}{2}\|\beta\|_1(\|\phi\|_1 + \|\rho\|_1) \quad (2.3)$$

$$\|F(\phi; \beta) - F(\phi; \hat{\beta})\|_1 \leq \frac{9A+1}{2}\|\beta - \hat{\beta}\|_1\|\phi\|_1^2 \quad (2.4)$$

The above inequalities are important in the convergence proofs presented in Sections 2 and 3. For example, from the inequalities (2.1)-(2.2) it is clear that $F(\rho)$ is uniformly Lipschitz in ρ , for ρ in a bounded set of the state space $C[0, A]$ (i.e, the Lipschitz constant L is independent of ρ), and $F(\rho, \beta)$ is continuous in β . We can deduce similar results from the inequalities (2.3)-(2.4) for the state space $C^1[0, A]$.

The main objective in this section is to establish convergence results taking into account that the different levels of regularity of solutions in Theorems A2 and A3 indicate possible types of approximations. In particular, we use here linear and cubic spline basis functions. The reason for using the linear splines is related to the identification problem and the regularity of the stickiness function, as we shall see in the following section.

We consider a sequence of spaces $X^N = \text{span}\{B_0^N, \dots, B_N^N\}$, where B_k^N denotes either linear or cubic spline basis functions on the interval $[0, A]$ (De Boor, 1987) and represent by π^N the usual interpolation operator on $C[0, A]$. In this setting, the approximate equation has the form

$$\frac{\partial \rho^N(t, x)}{\partial t} = \pi^N(F(\rho^N(t, x))) \quad (2.5)$$

with initial condition

$$\rho^N(0, x) = \pi^N(\rho_0(x)),$$

where as above

$$\rho^N(t, x) = \sum_{k=1}^N \alpha_k^N(t) B_k^N(x)$$

denotes the computational approximation. We begin our convergence analysis for the case of linear splines.

2.1. Interpolation using linear splines

We first note that the interpolation operators in the linear spline case satisfy the following:

(1L) $\pi^N: C[0, A] \rightarrow X^N \subset C[0, A]$ is a bounded linear operator, with operator norm $\|\pi^N\| = 1$, and

(2L) For any function $\phi \in C[0, A]$, $\pi^N \phi \rightarrow \phi$ as $N \rightarrow \infty$ (De Boor, 1987).

With these observations we are in a position to prove the following convergence

result.

Theorem 2.1. Suppose that $\rho_0 \in C[0, A]$, and that $\beta \in C([0, A] \times [0, A])$. Then, the semi-discrete solutions of equation (2.5) converges in $\|\cdot\|_0$ to the unique solution of (1.1), uniformly on the interval $[0, T_0]$.

Proof. We begin by writing (1.1) in integrated form:

$$\rho(t, x) = \rho_0(x) + \int_0^t F(\rho(t, x)) dt.$$

Likewise, we integrate (2.5) to obtain

$$\rho^N(t, x) = \rho_0^N(x) + \int_0^t \pi^N(F(\rho^N(t, x))) dt.$$

We remark that the existence theory in the Appendix applies to the semi-discrete version of the problem as well as the original one. Moreover, because the interpolation operators are uniformly bounded, a uniform bound in N exists for the semi-discrete solutions.

For simplicity we will use the notation $\rho(t) = \rho(t, \cdot)$.

For any $t \in [0, T_0]$,

$$\|\rho^N(t) - \rho(t)\|_0 = \|\rho_0^N - \rho_0 + \int_0^t [\pi^N(F(\rho^N(t))) - F(\rho(t))] dt\|_0$$

$$\begin{aligned}
&\leq \|\rho_0^N - \rho_0\|_0 + \int_0^t \|F(\rho^N(t)) - F(\rho(t))\|_0 dt \\
&+ \int_0^t \|\pi^N(F(\rho(t))) - F(\rho(t))\|_0 dt \\
&\leq \|\rho_0^N - \rho_0\|_0 + \int_0^t L \|\rho^N - \rho\|_0 dt \\
&+ \int_0^{T_0} \|\pi^N(F(\rho(t))) - F(\rho(t))\|_0 dt.
\end{aligned}$$

An application of the Gronwall inequality leads to

$$\|\rho^N(t) - \rho(t)\|_0 \leq \left(\|\rho_0^N - \rho_0\|_0 + \int_0^{T_0} \|\pi^N(F(\rho(t))) - F(\rho(t))\|_0 dt \right) e^{LT_0}$$

Letting $N \rightarrow \infty$ we have that

$$\|\rho_0^N - \rho_0\|_0 \rightarrow 0,$$

by condition (2L) above, and that

$$\int_0^{T_0} \|\pi^N(F(\rho(t))) - F(\rho(t))\|_0 dt \rightarrow 0$$

by condition (2L) and the dominated convergence theorem. Thus, we have

$$\|\rho^N(t) - \rho(t)\|_0 \rightarrow 0$$

uniformly in $t \in [0, T_0]$, as desired.

2.2. Interpolation using cubic splines

For cases in which the initial condition and the stickiness function are continuously differentiable, a higher order approximation method may be useful. In this subsection, we examine cubic B-spline collocation. We use π^N to represent the cubic B-spline interpolation operator, and we denote by X^N the span of the cubic B-spline basis functions. The subscript x indicates differentiation with respect to the x variable. In analogy with the linear spline case, we have

(1C) $\pi^N: C^1[0, A] \rightarrow X^N \subset C^1[0, A]$ is a bounded linear operator,

(2C) For any function $\phi \in C^1[0, A]$, $\pi^N \phi \rightarrow \phi$ in $C^1[0, A]$, as $N \rightarrow \infty$ (De Boor, 1987), and

(3C) there exists a number K such that $\|\pi^N\| \leq K$, for each N , where the operator norm is in $C^1[0, A]$.

Theorem 2.2. Suppose that $\rho_0 \in C^1[0, A]$, and that $\beta \in C^1([0, A] \times [0, A])$. Then the semi-discrete solutions of equation (2.5) converge in $\|\cdot\|_1$ to the unique solution of (1.1), uniformly in t on the interval $[0, T_1]$.

Proof. From the proof of Theorem 2.1, we know that

$$\sup_{x \in [0, A]} |\rho^N(t, x) - \rho(t, x)| \rightarrow 0 \quad \text{as } N \rightarrow \infty.$$

Hence, to show that

$$\|\rho^N(t, \cdot) - \rho(t, \cdot)\|_1 \rightarrow 0 \quad \text{as } N \rightarrow \infty,$$

we need only to show that

$$\sup_{x \in [0, A]} |\rho_x^N(t, x) - \rho_x(t, x)| \rightarrow 0 \quad \text{as } N \rightarrow \infty.$$

But

$$\rho_x(t, x) = \rho_{0x}(x) + \int_0^t \frac{\partial}{\partial x} F(\rho(t, x)) dt,$$

and

$$\rho_x^N(t, x) = \frac{\partial}{\partial x} \pi^N(\rho_0(x)) + \int_0^t \frac{\partial}{\partial x} \pi^N(F(\rho^N(t, x))) dt.$$

Hence, for any $x \in [0, A]$:

$$\begin{aligned} |\rho_x^N(t, x) - \rho_x(t, x)| &\leq \left| \frac{\partial}{\partial x} (\pi^N(\rho_0(x)) - \rho_0(x)) \right| \\ &+ \int_0^t \left| \frac{\partial}{\partial x} (\pi^N(F(\rho^N(t, x))) - \pi^N(F(\rho(t, x)))) \right| dt \\ &+ \int_0^t \left| \frac{\partial}{\partial x} (\pi^N(F(\rho(t, x))) - F(\rho(t, x))) \right| dt. \end{aligned}$$

An argument identical to that of the linear spline case yields:

$$\begin{aligned} |\rho_x^N(t, x) - \rho_x(t, x)| &\leq \left(\frac{\partial}{\partial x} |\pi^N(\rho_0) - \rho_0| \right. \\ &\left. + \int_0^{T_1} \left| \frac{\partial}{\partial x} (\pi^N(F(\rho(t, x))) - F(\rho(t, x))) \right| dt \right) e^{KL_1 T_1}. \end{aligned}$$

Hence again, an argument identical to that of the linear spline case yields:

$$\|\rho^N(t) - \rho(t)\|_1 \rightarrow 0,$$

as $N \rightarrow \infty$.

3. Approximation and the Inverse Problem

In this section we examine the problem of fitting the (approximate) solution of the model equation to data. There are many theoretical and computational difficulties in such a problem. An approach that has enjoyed a great deal of success is the least squares method, in which we seek to minimize

$$J(\beta) = \sum_{i,j} |\rho(t_i, x_j; \beta) - z_{i,j}|^2,$$

where $\{z_{i,j}\}$ denotes the observed size-density data and $\rho(t, x; \beta)$ denotes the dependence of the solution of (1.1) on the parameter β .

Difficulties arise due to the need for approximations in computing ρ and the amount of information we have concerning β . If we do not have a specified functional form for β , it may be desirable to minimize J over an infinite dimensional set of functions, which we will also have to approximate if we are to compute minimizers. In posing the fit-to-data problem in terms of a least squares cost to be minimized, the existence of a minimizer and convergence of minimizers under various approximations are guaranteed under quite general conditions. We shall

apply some abstract least squares results of Banks and Kunisch (1989) and Banks (1985) to the coagulation model problem. We begin by reviewing some of the relevant least squares theory.

3.1. Theoretical background

The problem is to minimize

$$J(q) = |Wu(q) - z|_Z^2 \quad (3.1)$$

over $q \in Q$, where $z \in Z$ is an observation, $u(q) \in H$ is the parameter dependent system state, and W is a mapping from H to Z . We also consider a sequence of approximations H^N and Q^M to H and Q , respectively. The approximate problem, then is to minimize

$$J^N(q) = |Wu^N(q) - z|_Z^2 \quad (3.2)$$

over $q \in Q^M$. Conditions which guarantee convergence of solutions $\hat{q}^{N,M}$ of (3.2) to solution $\hat{q}$ of (3.1) and the continuous dependence on observations are given in Banks and Kunisch (1989) and Banks (1985). We restate the convergence theorem here.

Theorem 3.1. Let the following assumptions hold:

- (i) The sets Q, Q^M lie in a metric space $\tilde{Q}$, with Q, Q^M compact in the $\tilde{Q}$ topology.
- (ii) If $q^M \in Q^M$ for each M , There exists $q^* \in Q$ and a subsequence q^{M_k} such that

$q^{M_k} \rightarrow q^*$ in the $\tilde{Q}$ topology.

(iii) For any $q \in Q$, there exists a sequence q^M such that $q^M \in Q^M$ and $q^M \rightarrow q$ in the topology $\tilde{Q}$.

(iv) For any $q^k \rightarrow q$ in $\tilde{Q}$, we have $Wu^N(q^k) \rightarrow Wu(q)$ in Z as $N, K \rightarrow \infty$.

(v) for each N , the mapping $q \rightarrow J^N(q)$ is continuous.

Then, there exist minimizers $\hat{q}^{M,N}$ of J^N over Q^M . Furthermore, any subsequence of $\hat{q}^{M,N}$ has a convergent subsequence and if $\bar{q}$ is the limit of such a subsequence, then it is a minimizer of J over Q .

3.2. Least squares and approximation in the algae problem

In our model, $\rho(\beta)$ is the parameter dependent state, with state space $H = C^1([0, T_0], C[0, A])$ or $C^1([0, T_1], C^1[0, A])$. Define the observation operator W by: $W\phi(t, x) = \{\phi(t_i, x_j)\}_{i=1, \dots, n}^{j=1, \dots, m} \quad \forall \phi \in H$. Note that W is continuous from either state space to $\mathbb{R}^{nm}$. Our objective is to minimize

$$J(\beta) = \sum_{i,j} |\rho(t_i, x_j; \beta) - z_{i,j}|^2 \quad (3.3)$$

over $\beta \in Q$, a compact set of $\tilde{Q}$. Problems that arise, as we have pointed out above, include the need for approximation. With the appropriate spline approximation spaces H^N and Q^M chosen, the approximate problem is to minimize

$$J^N(\beta) = \sum_{i,j} |\rho^N(t_i, x_j; \beta) - z_{i,j}|^2 \quad (3.4)$$

over $\beta \in Q^M$. For the choice of Q and Q^M we consider two “extreme” examples. One is a very simple case: β is a constant function. Here Q is taken to be a bounded set of nonnegative real numbers, and we can use $Q^M = Q$. In the other case, we assume only that β is a nonnegative, Lipschitz continuous function. In this case, we may take $Q = \{\beta \in C([0, A]^2): |\beta| \leq K, |\beta(x, y) - \beta(x', y')| \leq K|(x, y) - (x', y')|\}$ for some prespecified K . Since this set is infinite dimensional, approximations are needed to compute minimizers. In this case we may choose Q^M to be linear combinations of two-dimensional linear spline basis functions, incorporating the bounds of Q . Such a choice is readily seen (Banks and Kunisch, 1989) to satisfy the required hypotheses of Theorem 3.1. We now apply Theorem 3.1 to our model with the above approximations.

Theorem 3.2. Suppose that Q is a compact subset of $\tilde{Q} = C([0, A] \times [0, A])$, and suppose that $\rho_0 \in C[0, A]$. Suppose that Q^M is a sequence of approximations of Q that satisfy conditions (i), (ii), and (iii) of Theorem 3.1. Then the conclusions of Theorem 3.1 hold for the minimization problems (3.3) and (3.4) with the linear spline collocation approximation of ρ .

Proof. We first note that (v) holds from standard continuous dependence

results for ODE problems (Ladas and Lakshmikantham, 1972) together with the continuity of the observation operator W . It remains to show that (iv) holds for our linear spline collocation.

Let $\beta^M \rightarrow \beta$ in $\tilde{Q} = C([0, A] \times [0, A])$, and let

$$\dot{\rho}(\beta) = F(\rho, \beta)$$

and

$$\dot{\rho}^{N,M}(\beta^M) = \pi^N(F^M(\rho^{N,M}))$$

denote the differential equations associated with β and β^M , respectively, where $F^M(\rho) = F(\rho, \beta^M)$. Using the integrated form again, we see that

$$\begin{aligned} |\rho^{N,M}(t) - \rho(t)| &\leq |\rho_0^N - \rho_0| + \int_0^t |\pi^N(F^M(\rho^{N,M}(t))) - \pi^N(F^M(\rho(t)))| dt \\ &\quad + \int_0^t |\pi^N(F^M(\rho(t))) - \pi^N(F(\rho(t)))| dt + \int_0^t |\pi^N(F(\rho(t))) - F(\rho(t))| dt. \end{aligned}$$

From the inequality (2.2), it follows that $F(\rho, \beta)$ is continuous in β and since $\beta^M \rightarrow \beta$, β^M is a bounded sequence and one has from (2.1)-(2.2) that $F^M(\rho) = F(\rho, \beta^M)$ is Lipschitz in ρ uniformly in β^M . Hence, using these facts and a Gronwall inequality argument similar to that of the previous section gives us that

$$\rho^{N,M}(t, \cdot, \beta^M) \rightarrow \rho(t, \cdot, \beta) \quad \text{as } N, M \rightarrow \infty$$

uniformly in $t \in [0, T_0]$. Since W is continuous linear operator, we have that

$$W\rho^{N,M}(\beta^M) \rightarrow W\rho(\beta) \quad \text{as } N, M \rightarrow \infty.$$

In the case of cubic splines, more regularity is required of β .

Theorem 3.3. Suppose that Q is a compact subset of $\tilde{Q} = C^1([0, A] \times [0, A])$, and suppose that $\rho_0 \in C^1[0, A]$. Suppose that Q^M is a sequence of approximations of Q that satisfy conditions (i), (ii), and (iii) of Theorem 3.1. Then the conclusion of Theorem 3.1 holds for the minimization problems (3.3) and (3.4) with the cubic B-spline collocation approximation of ρ .

Proof. Again we need only to verify hypothesis (iv) of Theorem 3.1. Let $\beta^M \rightarrow \beta$ in the norm on $\tilde{Q}$. From the proof of Theorem 2.2 we have that:

$$\begin{aligned} |\rho_x^{N,M}(t, x) - \rho_x(t, x)| &\leq \left| \frac{\partial}{\partial x} \pi^N(\rho_0(x)) - \rho_{0x}(x) \right| \\ &+ \int_0^t \left| \frac{\partial}{\partial x} \pi^N(F^M(\rho^{N,M}(t, x))) - \frac{\partial}{\partial x} \pi(F^M(\rho(t, x))) \right| dt \\ &+ \int_0^t \left| \frac{\partial}{\partial x} \pi^N(F^M(\rho(t, x))) - \frac{\partial}{\partial x} \pi^N(F(\rho(t, x))) \right| dt \\ &+ \int_0^t \left| \frac{\partial}{\partial x} \pi^N(F(\rho(t, x))) - \frac{\partial}{\partial x} F(\rho(t, x)) \right| dt. \end{aligned}$$

Arguments similar to those in the previous proofs will give the result.

Compactness in $C^1([0, A] \times [0, A])$ will be more restrictive than compactness in $C([0, A] \times [0, A])$ (e.g., Uniform boundedness of second derivatives). However, in the simple example of constant β (taken from a bounded set) mentioned above,

the hypotheses (i), (ii), and (iii) of Theorem 3.1 (and, hence, Theorem 3.3) are easily seen to be satisfied.

4. Numerical Results

To test our schemes before applying them to experimental data, we used the following approach. One chooses parameter values for β , designated here by β^* and hereafter referred to as "true" values. Solutions of the resulting system are generated using the collocation method described in this paper (with cubic interpolation) and the package LSODE (obtained from NETLIB), a solver of an initial value problem for stiff or non stiff systems of first order differential equations based on the Gear method, is used to solve the resulting differential equation system. From these solutions a simulated data field is constructed, either an "ideal" case, which uses the computed solution as the data, or a "more realistic" case in which we add noise from a random number generator to the computed solution. We then use this data in the least squares setting described above. In all these tests the package LMDIF1 (obtained from NETLIB), a minimization routine that is based on the Levenberg-Marquardt method, was employed for optimization. We have used two forms of $\beta(x, y)$, $\beta(x, y) = \beta^0$ and $\beta(x, y) = \beta^0 + \beta^1(x + y)$ where β^0 , β^1 are constants. By restricting attention to bounded sets in β_0 and β_1 , we may invoke Theorem 3.3 for convergence of the minimizers. Tables 1-4 indicate how accurate the results are for the minimization problem convergence. We have

used as initial distribution $\rho_0(x) = be^{-ax}$ where a, b are constants.

Note that in Tables 3, 4 the model cannot fit the data exactly, because the data in these tables is not obtained directly from the model, but from noise added to the output of our model. For an additional illustration of the accuracy of the numerical results, we choose to present the values in row 1 of these tables graphically in Figs. 1-8. In Fig. 1, we present the graph of the density, $\rho(t, x)$, approximated by the collocation method using the estimated β value from the inverse method (using constant form of β). Fig. 2 presents the graph of the observations that are generated by adding noise to the collocation method approximations. In Fig. 3 is the difference between the collocation method using the approximated value of β and the observations. In Fig. 4 we show the graph of the density ρ for a arbitrarily chosen size versus time, superimposed on the graph of the observed density at that same size versus time. Figs. 5-8 show the analogous results of Figs. 1-4 using the form $\beta(x, y) = \beta^0 + \beta^1(x + y)$.

Table 1			
$\beta(x, y) = \beta^0$ with 10×10 data points			
Startup Value	β^0	β^{0^N}	No. of Iter.
1	0.3	0.3000000	18
0.6	2.0	1.9999999	21
0.5	0.8	0.7999999	17

Table 1. The observations used are the output of the collocation method for the "true value" β^0 . The approximated value of the parameter β^0 is β^{0^N} with the indicated number of iterations for convergence and startup value.

Table 2						
$\beta(x, y) = \beta^0 + \beta^1(x + y)$ with 10×10 data points						
S. V. for β^0	S. V. for β^1	β^0	β^1	β^{0^N}	β^{1^N}	No. of Iter.
0.1	1.0	0.9	0.1	0.900000	0.099999	132
1.0	2.0	0.5	3.0	0.499999	2.999999	52
0.5	0.3	0.2	0.8	0.199999	0.800000	49

Table 2. The same as Table 1 using the second form of β .

Table 3				
$\beta(x, y) = \beta^0$ with 10×10 data points and noise				
σ	Startup Value	β^0	β^{0^N}	No. of Iter.
0.3	0.5	0.2	0.201838	17
1.2	0.4	0.1	0.121024	17

Table 3. The observations used are the output of the collocation method with a normal distribution noise added using the indicated standard deviation σ . The rest of columns represent the same as Table 1.

Table 4							
$\beta(x, y) = \beta^0 + \beta^1(x + y)$ with 10×10 data points and noise							
σ	S. V. for β^0	S. V. for β^1	β^0	β^1	β^{0^N}	β^{1^N}	No. of Iter.
0.4	.6	.1	0.2	0.4	0.21685	0.38253	66
0.6	0.1	0.3	0.2	0.3	0.23123	0.26954	50

Table 4. The same as in Table 3 using the second form of β .

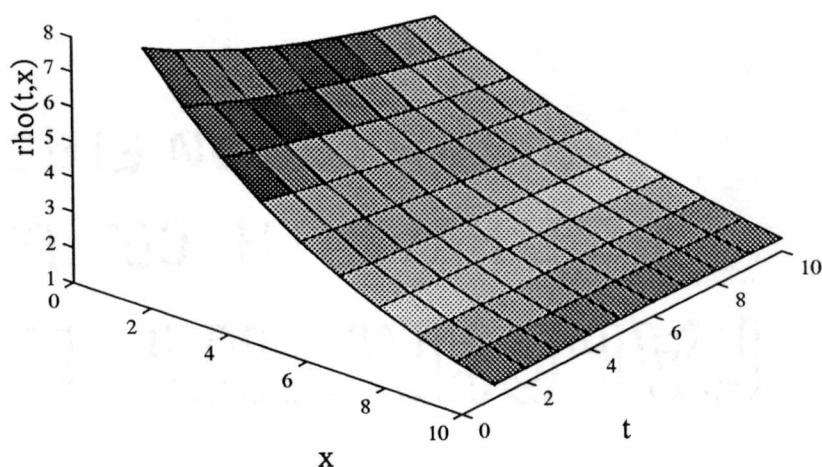


Fig. 1. The output of the collocation method using the approximation value β^{0N} in the first row of Table 3.

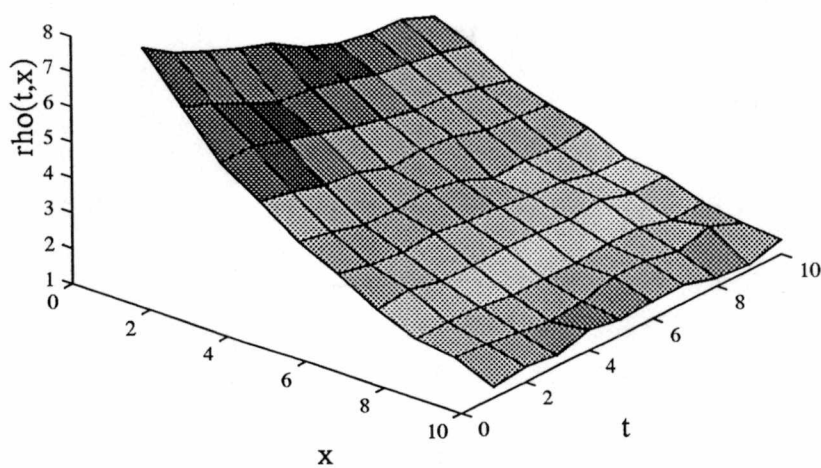


Fig. 2. The observations generated by adding noise to the collocation method output using the standard deviation in row 1 of Table 3.

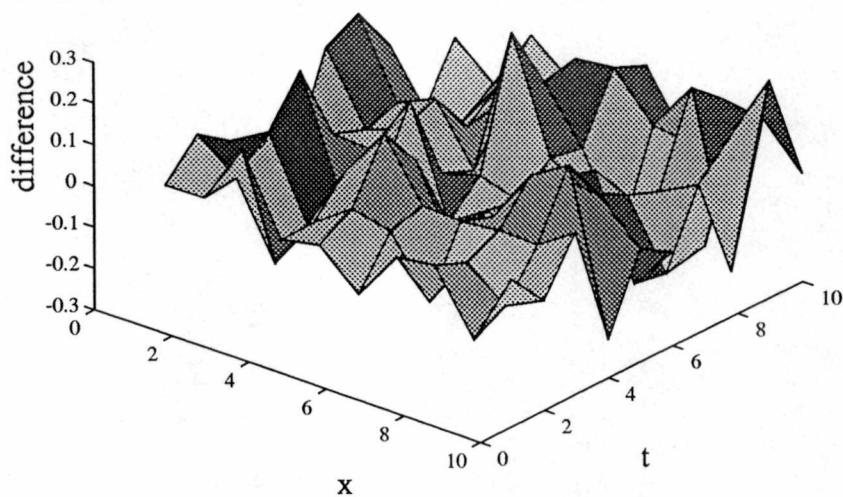


Fig. 3. The difference between the observations and the collocation method output. We note that the mean of the difference is approximately zero.

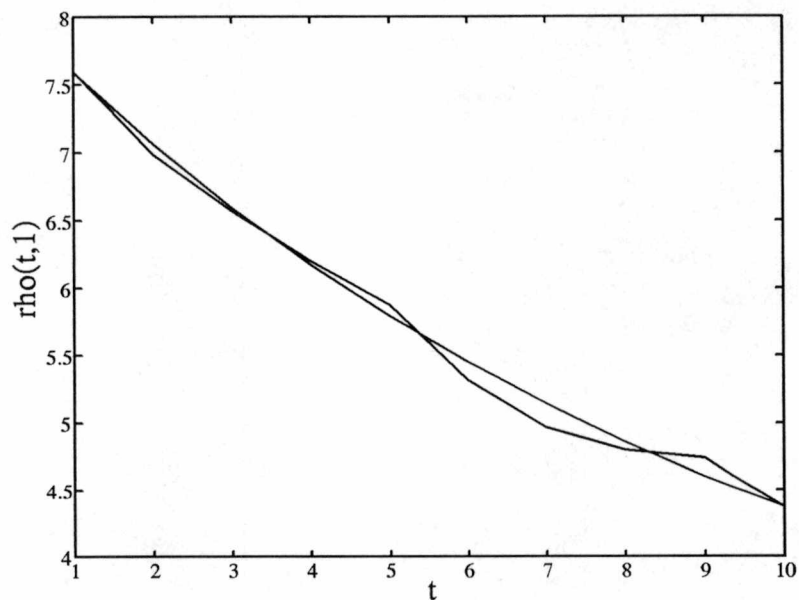


Fig. 4. The graph of the density at size 1 (this size was picked arbitrarily from the sizes 1-10, similar results hold for the other sizes) versus time. The two lines represent both, the observations and the output of the collocation method.

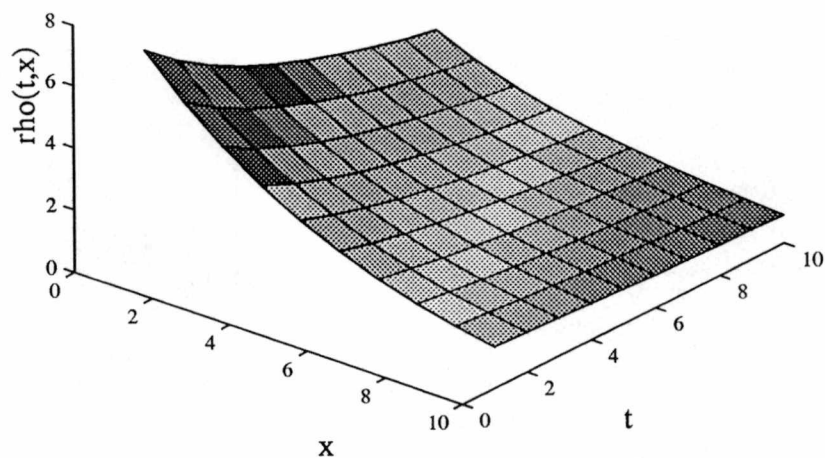


Fig. 5. The analogue of Fig. 1. but for the second form of β ($\beta(x, y) = \beta_0 + \beta_1(x + y)$) using the parameter values in row 1 of Table 4.

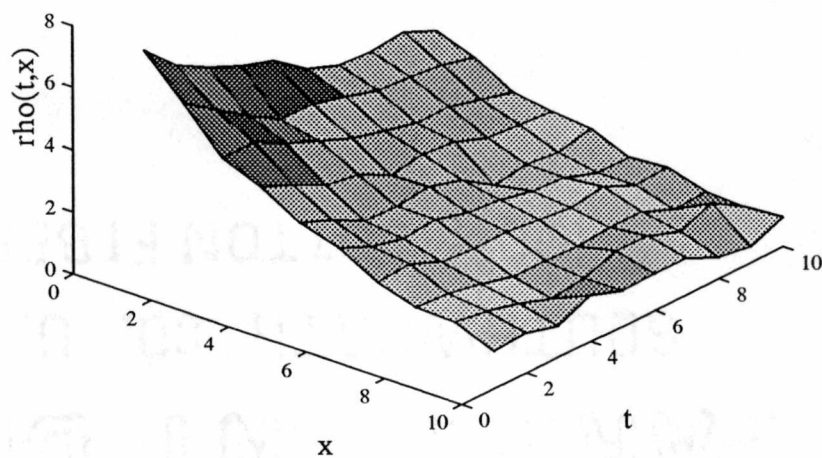


Fig. 6. The analogue of Fig. 2. but for the second form of β ($\beta(x, y) = \beta_0 + \beta_1(x + y)$) using the parameter values in row 1 of Table 4.

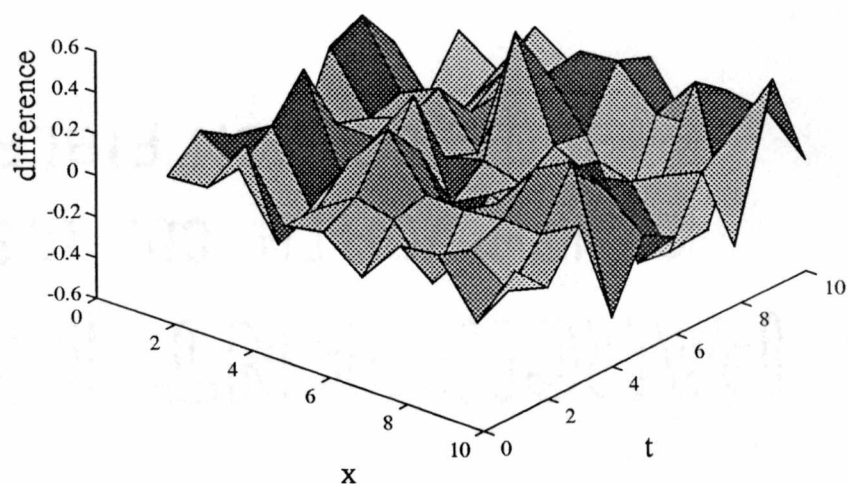


Fig. 7. The analogue of Fig. 3. but for the second form of β ($\beta(x, y) = \beta_0 + \beta_1(x + y)$) using the parameter values in row 1 of Table 4. We note that the mean of the difference is approximately zero.

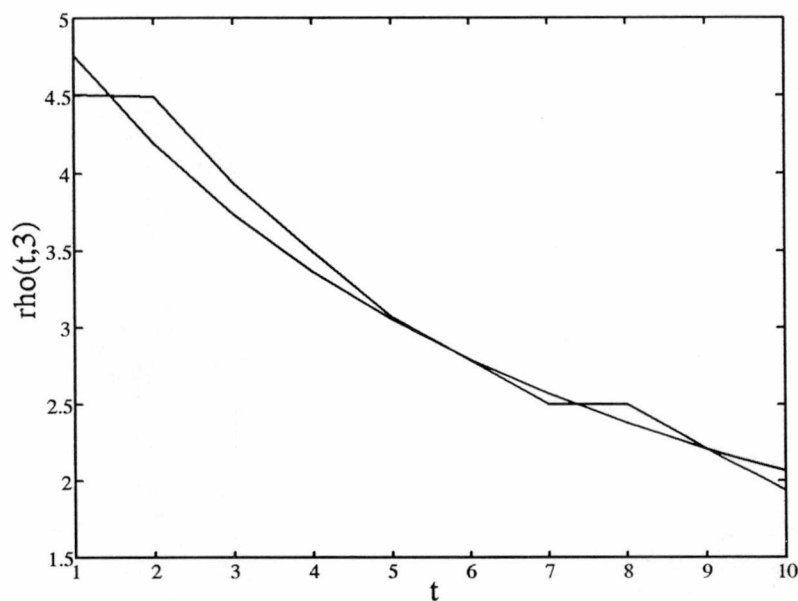


Fig. 8. The analogue of Fig. 4. but for the second form of β ($\beta(x, y) = \beta_0 + \beta_1(x + y)$) using the parameter values in row 1 of Table 4.

5. Concluding Remarks

A classical coagulation model and the well known collocation numerical technique blend into an attractive scheme for the study of aggregation of algae in the oceans. In this paper, we have focused on the mathematical justification of numerical convergence properties and on development of a procedure to estimate stickiness, a fundamental parameter in the coagulation kernel.

The collocation method is a very simple technique to implement numerically, and this is the principal reason why it has emerged as a very attractive method for integrodifferential equations. Among other commonly used techniques, such as Galerkin method and the method of moments, only the collocation method does not require extensive integral evaluations.

For the inverse method Tables 1,2 indicate the accuracy of the method if the observed data is attained, and Tables 3,4 indicate that in all these tests this method converged to a minimizer that fit the observed data well even though the data is not attained by our model (since we added noise to it). Hence from these numerical tests one expects that this method will work well for real data.

The utility of the classical coagulation model for studying aggregation in algal communities remains to be validated. As an initial step in this process, the development and establishment of the convergence properties of the numerical procedure is demonstrated in this paper. The results are presented here in a simple

setting where relevant biological oceanography has been suppressed.

There are more sophisticated models that include biological processes in aggregation (see Part III). Such models take the form

$$\begin{aligned}\frac{\partial \rho(t, x)}{\partial t} &= F(\rho(t, x)) - p \frac{\rho(t, x)}{\rho(t, x) + k(x)} Z(t) - G(x, \rho(t, x)) \\ \frac{\partial Z(t, x)}{\partial t} &= peZ \frac{\rho(t, x)}{\rho(t, x) + k(x)} - mZ(t)\end{aligned}$$

with initial conditions:

$$\rho(0, x) = \rho_0(x) \text{ and } Z(0) = Z_0.$$

Here, Z represents the density of the grazers feeding on aggregates of size x at time t , and G is a function that represents the loss of aggregates due to sinking. The function k is the positive half saturation constant that depends on the aggregate size. The constants p and e are the ingestion rate and the assimilation efficiency, and m is the mortality constant. The biology of the algae is handled according to an individual model that describes the growth of a single cell. This model takes the following form:

$$\frac{dv}{dt} = \frac{N}{N + K_N} (av^{\frac{2}{3}} - bv)$$

with initial condition:

$$v(0) = v_{min}$$

where v is the volume of the cell (μm^3) and N (μM) represents the nutrient abundance and a , b are growth and maintenance rates of the cell. We expect to be

able to obtain results similar to those of the previous sections, under reasonable assumptions on G and k .

Acknowledgments

We are grateful to Dr. Lou Gross for his useful comments and his help in obtaining the graphs in this paper. This work was supported by the Office of the Naval Research Contract N00014-92-J1139, the National Science Foundation Grant USE-9150354 and the Air Force Office of Scientific Research Grant AFOSR-91-0021 to the University of Tennessee at Knoxville.

Appendix: Existence, Uniqueness, and Regularity

We take a rather standard approach for ordinary differential equations in Banach spaces and first restate a theorem from Ladas and Lakshmikantham (1972) (page 129).

Theorem A.1. Let X be a Banach space, and suppose that $t_0 \in \mathbb{R}$, $u_0 \in X$, and $a, b > 0$. Let $I = [t_0 - a, t_0 + a]$, and $S = \{u : \|u - u_0\| \leq b\}$. Define the rectangle $R_0 = I \times S \subset \mathbb{R} \times X$. Let $f : R_0 \rightarrow X$ be continuous in t for each fixed u . Assume that $\|f(t, u)\| \leq M$ for $(t, u) \in R_0$ and $\|f(t, u_1) - f(t, u_2)\| \leq K\|u_1 - u_2\|$ for $(t, u_1), (t, u_2) \in R_0$ where K and M are nonnegative constants, with $aM \leq b$.

Then there exists one and only one (strongly) continuously differentiable function $u(\cdot) : I \rightarrow X$ satisfying

$$\frac{du(t)}{dt} = f(t, u(t)), \quad |t - t_0| \leq a$$

and

$$u(t_0) = u_0.$$

Using the above theorem and letting $X = C[0, A]$, and we can prove the following:

Theorem A.2. Suppose that $\rho_0 \in C[0, A]$, and that $\beta \in C([0, A] \times [0, A])$. Then, there exists a $T_0 > 0$ and a unique function $\rho \in C^1([0, T_0]; C[0, A])$ satisfying $\rho(0) = \rho_0$ and Eq. (1.1) on $[0, T_0]$.

Proof. For any fixed positive constant b let S be defined as in the theorem above, Choose $T_0 = \frac{2}{3A\|\beta\|_0 b}$, define $R_0 = J \times S = [0, T_0] \times \{\rho \in X : \|\rho - \rho_0\|_0 \leq b\}$.

Clearly $F(\rho(t, \cdot)) : R_0 \rightarrow C[0, A]$ is continuous in t for each fixed ρ and satisfies $\|F(\rho)\|_0 \leq M$ for $(t, u) \in R_0$ and a positive constant M satisfying $M = \frac{3A}{2}\|\beta\|_0 b^2$. $T_0 M = b$; hence, it remains to show that $F(\rho)$ is Lipschitz with respect to ρ on R_0 in order to establish the result. For any $\phi, \rho \in R_0$ we have:

$$|F(\phi) - F(\rho)| \leq \frac{1}{2} \int_0^x \beta(x-y, y)(\phi(t, x-y)\phi(t, y) - \phi(t, y)\rho(t, x-y))$$

$$\begin{aligned}
& + |\phi(t, y)\rho(t, x - y) - \rho(t, x - y)\rho(t, y))dy| \\
& + |\phi(t, x) \int_0^A \beta(x, y)\phi(t, y)dy - \phi(t, x) \int_0^A \beta(x, y)\rho(t, y)dy \\
& + \phi(t, x) \int_0^A \beta(x, y)\rho(t, y)dy - \rho(t, x) \int_0^A \beta(x, y)\rho(t, y)dy| \\
& \leq \frac{1}{2}\|\beta\|_0 \int_0^x \left(|\phi(t, y)| |\phi(t, x - y) - \rho(t, x - y)| \right. \\
& + |\rho(t, x - y)| |\phi(t, y) - \rho(t, y)| \Big) dy \\
& + \|\beta\|_0 |\phi(t, x)| \int_0^A |\phi(t, y) - \rho(t, y)| dy \\
& + \|\beta\|_0 |\phi(t, x) - \rho(t, x)| \int_0^A |\rho(t, y)| dy \\
& \leq \frac{A}{2}\|\beta\|_0 \left((\|\phi\|_0 \|\phi - \rho\|_0 + \|\rho\|_0 + \|\phi - \rho\|_0) \right) \\
& + A\|\beta\|_0 \left(\|\phi\|_0 \|\phi - \rho\|_0 + \|\phi - \rho\|_0 \|\rho\|_0 \right) \\
& \leq \frac{3A}{2}\|\beta\|_0 \left(\|\phi\|_0 + \|\rho\|_0 \right) \|\phi - \rho\|_{C^0} \leq L\|\phi - \rho\|_0.
\end{aligned}$$

Taking the supremum over all $x \in [0, A]$ we get:

$$\|F(\phi) - F(\rho)\|_0 \leq L\|\phi - \rho\|_0.$$

Letting $X = C^1[0, A]$ we can prove the following:

Theorem A.3. Suppose that $\rho_0 \in C^1[0, A]$, and that $\beta \in C^1([0, A] \times [0, A])$. Then, there exists a $T_1 > 0$ and a unique function $\rho \in C^1([0, T_1]; C^1[0, A])$ satisfying $\rho(0) = \rho_0$ and Eq. (1.1) on $[0, T_1]$.

Proof. For any fixed positive constant b let S be defined as in the theorem above, Choose $T_1 = \frac{2}{(9A+1)\|\beta\|_1 b}$, define $R_0 = J \times S = [0, T_1] \times \{\rho \in X : \|\rho - \rho_0\|_1 \leq b\}$.

Clearly $F(\rho(t, \cdot)) : R_0 \rightarrow C^1[0, A]$ is continuous in t for each fixed ρ .

Note that:

$$\begin{aligned} \frac{\partial}{\partial x} F(\rho(t, x)) &= \frac{1}{2} \beta(0, x) \rho(t, 0) \rho(t, x) + \frac{1}{2} \int_0^x \left(\beta_x(x-y, y) \rho(t, x-y) \rho(t, y) \right. \\ &\quad \left. + \beta(x-y, y) \rho_x(t, x-y) \rho(t, y) \right) dy \\ &\quad - \rho_x(t, x) \int_0^A \beta(x, y) \rho(t, y) dy - \rho(t, x) \int_0^A \beta_x(x, y) \rho(t, y) dy \end{aligned}$$

Hence, it is easy to show that $\|F(\rho)\|_1 \leq M$ on R_0 with $M = \frac{9A+1}{2} \|\beta\|_1 b^2$; clearly $T_1 M = b$.

Let $\phi, \rho \in C^1[0, A]$ then, from the previous theorem, we have that for any $x \in [0, A]$:

$$|F(\phi) - F(\rho)| \leq L \|\phi - \rho\|_0 \leq L \|\phi - \rho\|_1.$$

Hence, to show that $F(\rho)$ is Lipschitz, it needs to be demonstrated that for any $x \in [0, A]$:

$$\left| \frac{\partial}{\partial x} F(\rho) - \frac{\partial}{\partial x} F(\phi) \right| \leq \hat{L} \|\rho - \phi\|_1.$$

Similar techniques as in the proof of the previous theorem will lead to:

$$\left| \frac{\partial}{\partial x} F(\rho) - \frac{\partial}{\partial x} F(\phi) \right| \leq \frac{6A+1}{2} \|\beta\|_1 \left(\|\phi\|_1 + \|\rho\|_1 \right) \|\phi - \rho\|_1 = \hat{L} \|\rho - \phi\|_1.$$

Hence,

$$\begin{aligned}\|F(\phi) - F(\rho)\|_1 &\leq (L + \hat{L})\|\phi - \rho\|_1 \\ &\leq \frac{9A+1}{2}\|\beta\|_1(\|\phi\|_1 + \|\rho\|_1)\|\phi - \rho\|_1 = L_1\|\phi - \rho\|_1.\end{aligned}$$

and we have that F is Lipschitz in ρ , which concludes the proof in light of Theorem A.1.

In the next theorem we will show that under certain (physically natural) assumptions on ρ_0 and β we have a conservation of mass law and a global solution of (1.1).

Notice that the assumption on ρ_0 implies that particle size is not smaller than some (positive) minimum size. The first assumption on β implies that the probability of an aggregate of size x sticking to an aggregate of size y is the same as that of an aggregate of size y sticking to an aggregate of size x , and the second assumption implies that there exist a maximum aggregate size A . This assumption has been shown to hold in some cases (Riebesell, 1991).

Theorem A.4. Suppose that $\rho_0 \in C[0, A]$ satisfies $\rho_0(x) \geq 0 \ \forall x \in [0, A]$ and $\rho_0(x) = 0$ for $x < x_{min}$, where $x_{min} \in [0, A]$ is a positive constant, and that $\beta \in C([0, A] \times [0, A])$ satisfies $\beta(x, y) = \beta(y, x)$ and $\beta(x, y) = 0$ if $(x + y) > A$. Then, there exists a unique function $\rho \in C^1([0, \infty); C[0, A])$ satisfying the following: $\rho(t, x) \geq 0 \ \forall x \in [0, A]$ and $\forall t \in [0, \infty)$ $\frac{d}{dt} \int_0^A x \rho(t, x) dx = 0$ and ρ is a

global solution of (1.1).

Proof. To show that $\rho(t, x) \geq 0$ just notice that if $\rho(t, x) = 0$ for some $x \in [0, A]$ then $\dot{\rho}(t, x) \geq 0$ hence the plane $z = 0$ (in the x, y, z coordinates) is invariant so the solution cannot cross this plane.

Next we show that the following conservation of mass law is satisfied:

$$\frac{d}{dt} \int_0^A x \rho(t, x) dx = \int_0^A x \frac{d\rho(t, x)}{dt} dx = 0 .$$

From Eq. (1.1) we have:

$$\begin{aligned} \int_0^A x \frac{d\rho(t, x)}{dt} dx &= \int_0^A \frac{x}{2} \int_0^x \beta(x-y, y) \rho(t, x-y) \rho(t, y) dy dx \\ &\quad - \int_0^A x \rho(t, x) \int_0^A \beta(x, y) \rho(t, y) dy dx . \end{aligned}$$

Starting with the first term on the right hand side of the above equation then reversing the order of integration we find

$$\begin{aligned} &\int_0^A \frac{x}{2} \int_0^x \beta(x-y, y) \rho(t, x-y) \rho(t, y) dy dx \\ &= \int_0^A \int_y^A \frac{x}{2} \beta(x-y, y) \rho(t, x-y) \rho(t, y) dx dy . \end{aligned}$$

Using the change of variables $z = x - y$ and the assumptions on β we get

$$\begin{aligned} &\int_0^A \frac{x}{2} \int_0^x \beta(x-y, y) \rho(t, x-y) \rho(t, y) dy dx \\ &= \int_0^A \frac{y}{2} \rho(t, y) \int_0^A \beta(z, y) \rho(t, z) dz dy \\ &\quad + \int_0^A \int_0^A \frac{z}{2} \beta(z, y) \rho(t, z) \rho(t, y) dz dy \\ &= \int_0^A x \rho(t, x) \int_0^A \beta(x, y) \rho(t, y) dy dx . \end{aligned}$$

Hence, this proves the conservation of mass result.

From the assumption that $\rho_0 = 0 \quad \forall x \in [0, x_{min}]$, we get that $\rho(t, x) = 0 \quad \forall x \in [0, x_{min}]$. Hence using the conservation of mass result we have:

$$\int_0^A x \rho(t, x) dx = \int_{x_{min}}^A x \rho(t, x) dx = \int_{x_{min}}^A x \rho_0 dx$$

From the fact that $\rho(t, x) \geq 0$ we can deduce the following:

$$\int_0^A \rho(t, x) \leq E;$$

hence, we can show that:

$$\begin{aligned} \|\dot{\rho}(t, \cdot)\|_0 &\leq \frac{M}{2} \|\rho(t, \cdot)\|_0 \int_0^x \rho(t, y) dy + M \|\rho(t, \cdot)\|_0 \int_0^A \rho(t, y) dy \\ &\leq \frac{3ME}{2} \|\rho(t, \cdot)\|_0. \end{aligned}$$

Using the comparison theorem in Ladas and Lakshmikantham (1972) (page 161)

with the following scalar differential equation

$$\dot{s} = \frac{3ME}{2} s,$$

with initial condition:

$$s(0) = \|\rho_0\|_0,$$

we conclude that ρ is a global solution of (1.1).

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Part III

THE ROLE OF AGGREGATE FORMATION IN PHYTOPLANKTON BLOOM DYNAMICS*

Abstract - Aggregate formation, the genesis of larger particles from the collisions of smaller ones, is fundamental to many biological processes in the ocean. Because large particles generally sink faster than small ones, aggregate formation can be important in increasing mean particle size and accelerating the flux of biogenic matter from the ocean's surface to the deep sea. It also may limit phytoplankton population size by increasing loss rates over monthly and seasonal time scales. Although algal species are most directly affected by the coagulation process, the oceanographic food web is also impacted, at least indirectly, by the aggregation process. To better understand the role of aggregate formation within phytoplankton bloom dynamics, we investigate the dynamics of a structured algal population in the context of a food-chain model. Although the model is generic in character, we focus specifically on diatoms for parameterization. The food-chain model incorporates nutrient and grazing dynamics, and the model of the phytoplankton assemblage includes individual diatom life history describing cell growth and reproduction. The simulations demonstrate that the presence of grazers influence algal population dynamics by generating cyclic fluctuations for aggregate densi-

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ties and changing the length of the bloom period by enhancing loss rates. The number of living cells in aggregates is important to an understanding of aggregate dynamics because increasing numbers of live cells enhance aggregation and hence phytoplankton losses. Under certain conditions aggregate formation can be a quantitatively significant loss process within marine phytoplankton populations.

1. Introduction

Oceanic aggregates are composed of a variety of biologically derived organic materials, including algal cells, fecal pellets, and animal feeding structures, such as mucus nets from pteropods and larvacean feeding structures (Alldredge and Silver, 1988). Aggregates can be relatively large when compared to the size of a single cell. For example, aggregates more than 1 *mm* in length are frequently observed in the ocean after algal blooms (Trent et al., 1978; Alldredge and Gotschalk, 1988a,b; Kiorboe et al., 1990). Marine aggregates have been observed to increase in size with increasing depth (Kranck and Milligan, 1990). A number of models have suggested that aggregate formation is a quantitatively significant loss process (Jackson, 1990; Hill, 1992; Jackson and Lochmann, 1992), and recent studies in the North Sea reinforce the suggestion that coagulation is an important process for determining the fate of organic matter produced by phytoplankton blooms (Riebesell, 1991a,b).

Inherent to the aggregation process is the concept of "stickiness" : when two particles collide, there is a positive probability they will adhere to form larger par-

ticles. Laboratory studies (Kiorboe et al., 1990) and field experiments (Alldredge et al. personal communication) have shown that algal cells have a positive probability to coagulate when they collide. However, the principal factors governing stickiness remain unclear. One hypothesis is that algal stickiness is a function of available nutrients. Kiorboe et al., (1990) showed that phytoplankton stickiness increased when nutrients were depleted from the medium. However, recent experiments have suggested that there is a weak relationship between nutrient concentration of the medium and the probability of one cell's sticking to another (Alldredge et al. personal communication).

The models of Jackson (1990), Hill (1992) and Jackson and Lochmann (1992) focused primarily on the role of physical processes in the coagulation of phytoplankton. These models parameterized algal growth as being either constant (Jackson 1990) or nutrient and irradiance dependent (Jackson and Lochmann, 1992). The conclusions from these models were that coagulation can limit phytoplankton yields and accelerate the removal of senescent cells by aggregating them into larger, more rapidly sinking particles. Hill (1992) suggested that only in regions which attain high densities of phytoplankton can random collision occur frequently enough to produce significant aggregate formation and high rates of vertical flux. Although these models revealed the importance of coagulation in limiting phytoplankton population size, they have not included detailed biological description of the phytoplankton or the role of resource-consumer interactions.

This paper focuses on algal population dynamics and presents a food-chain

model in which the effects of biological processes at the individual level are incorporated. Growth of phytoplankton cells is modeled as a function of cell volume, and the dynamics of phytoplankton, zooplankton, and nutrients are represented in a simple resource-consumer model. Understanding the interactions between food chain dynamics and coagulation can clarify the role of the coagulation in limiting phytoplankton populations. Aggregation should be especially important in regimes with high nutrients and low zooplankton densities (Jackson and Lochmann, 1992). This development concentrates on the phytoplankton community by including detailed representations of the biological aspects of the algal population and employing generic, nonstructured descriptions for nutrient and grazer dynamics. The lack of structure in the zooplankton community is an initial approximation, but this level of resolution allows us to infer to the importance of grazing.

2. Model Description and Methodology

The food-chain model consists of an individual-based model of an algal cell, a coagulation model describing the aggregation process, a representation of nutrient dynamics and a grazer model (Fig. 1).

2.1. Individual cell model

If v is the volume of a single diatom cell, then the rate of volume change

with respect to time is taken to be the uptake rate minus the maintenance rate. Both physiological processes depend on the availability of nutrients. Cell growth is assumed to be proportional to surface area with the constant of proportionality a ($\mu\text{m d}^{-1}$). The maintenance costs or respiration rate is assumed proportional to the cell volume with constant of proportionality b (d^{-1}). Thus, we assume that

$$\frac{dv}{dt} = \begin{cases} \frac{N-N_T}{k_N+N-N_T}(av^{\frac{2}{3}} - bv) & N > N_T \\ 0 & N \leq N_T \end{cases} \quad (2.1)$$

with the initial condition

$$v(0) = v_{\min}.$$

In (2.1), N is the concentration of the limiting nutrient, N_T is the threshold level of nutrient at which cell physiological function ceases and the cell is in a "resting state". The constant k_N is the half saturation constant for the limiting nutrient. In the cell's life history, each cell is formed with a fixed volume ($v_{\min}$), grows according to the above model and asexually divides when its volume doubles.

Because most models do not represent growth as a function of volume, not all parameter values are readily available from literature; hence, we utilize the reported values of maintenance rate b and estimate the value of a from solutions to the model. When nutrients are not limiting, then (2.1) can be approximated by the von Bertalanffy model

$$\frac{dv}{dt} = av^{\frac{2}{3}} - bv, \quad (2.2).$$

with initial condition

$$v(0) = v_{min}.$$

The exact solution of (2.2) is given by

$$v(t) = \left(\frac{a}{b} - \frac{a - bv_{min}^{\frac{1}{3}}}{b} e^{\frac{-bt}{3}} \right)^3.$$

If the time required for a diatom cell to double its volume and divide under abundant nutrients is $\hat{t}$ (i.e., $v(\hat{t}) = 2v_{min}$), then

$$a = \frac{v_{min}^{\frac{1}{3}}(2^{\frac{1}{3}} - E)}{\frac{1-E}{b}}$$

where

$$E = e^{\frac{-b\hat{t}}{3}}.$$

Fig. 2 indicates the increase of v with respect to time using different values of the nitrogen N with value of b taken as $b = 0.0084$ (d^{-1}) as estimated by Lancelot (1991) for diatoms. The parameter a is calculated by the above method with an assumed doubling time ($\hat{t}$) of 1 day. Fig. 2B and Fig. 2C are analogous to Fig. 2A except different b values found in the literature $b = 0.04$ (d^{-1}) (EPA, 1985) and $b = 0.1$ (d^{-1}) (Jørgensen, 1979) are employed. Fig. 3 represents the individual model output for the above three values of b and a fixed nutrient value and indicates that the difference in the life history of the cell (over the range $v_{min} \leq v \leq 2v_{min}$) is negligible among the various choices of b . Hence, we arbitrarily set $b = 0.0084$ (d^{-1}) in all other simulations.

The individual model (2.1) is based on organismal size and is closely related to the classical von Bertalanffy equation (Kooijman, 1993) except that nutrients are modeled differently. In the von Bertalanffy representation, the ultimate cell size and the growth rate are functions of nutrient density, whereas in the model utilized here only the rate of growth is affected by the nutrient level. This allows for the existence of a resting stage at low nutrient levels that cannot result from the von Bertalanffy representation.

2.2. Grazer-aggregate model

If $\rho(t, x)$ is the density of the aggregates with volume x at time t , then the number of aggregates in the range x and $x + dx$ is ρdx . To describe the rate of change of ρ due to coagulation, we have used the equation employed by Smoluchowski (1917) to investigate the kinetics of the coagulation of colloidal solutions, by Gelbard and Sienfeld (1978) to describe the coagulation of homogeneous particles and by Jackson and Lochmann (1992) to describe the aggregation of phytoplankton cells. This equation is as follows:

$$\begin{aligned} \frac{\partial \rho(t, x)}{\partial t} = & \frac{1}{2} \int_0^x \alpha(x-y, y) \beta(x-y, y) \rho(t, x-y) \rho(t, y) dy \\ & - \rho(t, x) \int_0^A \alpha(x, y) \beta(x, y) \rho(t, y) dy = F(\rho(t, x)) \end{aligned} \quad (2.3)$$

where $\beta(x, y)$ is the coagulation kernel for collision of two particles, one with volume x and the other with volume y and $\alpha(x, y)$ is the probability that they stick after colliding (e.g., Pruppacher and Klett, 1980). The first term in (2.3) expresses the rate at which collisions occur to form new particles with volume between x and $x + dx$ while the second term expresses the rate at which collisions cause particles to be lost from that size class due to aggregation with other particles from the same interval.

The coagulation kernel $\beta(x, y)$ consists of two parts, both of which are symmetric and non-negative (Riebesell and Gladrow, 1992). The first part $\beta^s(x, y)$ is due to shear flow (McCave, 1984):

$$\beta^s(x, y) = 0.163 \left(\frac{\epsilon}{\nu} \right)^{\frac{1}{2}} (d_x + d_y)^3 EC_{x,y},$$

where ϵ is the energy dissipation rate ($10^{-6} m^2 s^{-3}$), ν is the kinematic viscosity ($1.43 \times 10^{-6} m^2 s^{-1}$), d_x is the diameter of particle of volume x and d_y is the diameter of a particle of volume y , and $EC_{x,y}$ is the efficiency (i.e., the probability that two particles in close proximity come in direct contact). The diameter d_x is given by $d_x = 2 \times \left(\frac{3x}{4\pi} \right)^{\frac{1}{3}}$ and d_y is represented by a similar function. The second part stems from the differential settling (McCave, 1984):

$$\beta^d(x, y) = \frac{\pi(d_x + d_y)^2}{4} |w_x - w_y| (EC_{x,y} + ED_{x,y})$$

where w_x and w_y are settling velocities of particles with volume x and y , $ED_{x,y}$

is the diffusion efficiency (McCave, 1984), which has been neglected in the present model (diffusion is negligible for particles $\gg 1\mu m$). The contact efficiency $EC_{x,y}$ for differential settling (Pruppacher and Klett, 1980) is of the form:

$$EC_{x,y} = \frac{(d_{min}/d_{max})^2}{2(1 + d_{min}/d_{max})^2}$$

where $d_{min} = \min(d_x, d_y)$ and $d_{max} = \max(d_x, d_y)$. In order to apply contact efficiency to both collision mechanisms, a function approximating theoretical contact efficiency data for shear flow as presented in Pruppacher and Klett (1980) was introduced:

$$EC_{x,y}(d_{min}/d_{max}) = EC_0 \exp\left(-\frac{0.1}{d_{min}/d_{max}}\right)$$

where $EC_0 = 1/\exp(-0.1)$. This function yields contact efficiencies approaching unity for $d_{min}/d_{max} > 0.1$ and exponentially decreasing contact efficiencies for $d_{min}/d_{max} < 0.1$.

If aggregates of size x sink at velocity $w(x)$, then adding particle loss due to sinking in the equation results in

$$\frac{\partial \rho(t, x)}{\partial t} = F(\rho(t, x)) - \rho(t, x) \frac{w(x)}{D} \quad (2.4)$$

where D is the depth of the surface layer. It is assumed that if a cell sinks from the surface layer it cannot re-enter. The settling velocity of an aggregate of radius $R = (\frac{3x}{4\pi})^{\frac{1}{3}}$, is given by

$$w(x) = f_\rho \xi R^{1.17}. \quad (2.5)$$

(Jackson, 1989) where the constants f_p is the fall scale parameter and ξ is a curve fit parameter whose values are given in Table 1. Eq. (2.5) is consistent with the settling velocities of millimeter-diameter particles and aggregates (Alldredge and Gotschalk, 1988a,b).

To investigate the effects of grazing, we employ a generic grazing representation for the dynamics of zooplankton (Scheffer, 1991; Steele and Henderson, 1992). We model grazing not only on single cells but also on aggregates of a prescribed size. The zooplankton population model initially has the form

$$\frac{dZ}{dt} = p \delta \frac{\int_0^A f(x) \rho(t, x) dx}{\int_0^A f(x) \rho(t, x) dx + k_p} Z - mZ \quad (2.6)$$

where Z is the density of the grazers. In the first term, a zooplankter is assumed to have a rate of ingestion p with an assimilation efficiency δ . Therefore, the total uptake of the zooplankton population is the instantaneous ingestion per individual times the density of the zooplankton at that time. The function $f(x)$ was added to reflect the probability of an individual zooplankter ingesting an aggregate of size x . Because an animal can ingest only an aggregate of maximum size x_{max} , then $f(x) = 0$ for $x > x_{max}$. Fig. 4 presents the graph of $f(x)$ versus x when $x_{max} = 0.02 \text{ mm}^3$ (Lancelot et al., 1991). We have assumed that the probability of a zooplankter ingesting a single cell is 1 and the probability decreases (using a second degree polynomial) as the size of the aggregate increases.

The second term in (2.6) represents the loss of zooplankton due to a constant

mortality rate, m . Multiplication by the zooplankton population density yields the total population loss due to mortality. In (2.6), k_p is the trophic response half saturation constant. Adding the loss of aggregates due to grazing to Eq. (2.4) yields

$$\frac{\partial \rho(t, x)}{\partial t} = F(\rho(t, x)) - \rho(t, x) \frac{w(x)}{D} - p \frac{f(x) \rho(t, x)}{\int_0^A f(x) \rho(t, x) dx + k_p} Z. \quad (2.7)$$

Eqs. (2.6) and (2.7) coupled with (2.1) form the aggregation, algal and zooplankton community model without nutrient dynamics. To compute the change of dissolved nutrient with respect to time, the carbon mass of a cell with radius r is given by

$$\phi = c \times r^{2.28}$$

where c is constant (Mullin et al., 1966). Its nitrogen mass is the carbon content divided by the Redfield Ratio, $m_0 = \frac{\phi}{6}$. The change in nitrogen mass of each cell is calculated using the change in radius and the above relationships. Nitrogen is conserved, so integration over the change of nitrogen mass in each living cell leads to the total change in the dissolved pool.

2.3. Numerical procedure

To solve equation (2.7) we use the spline-based collocation method (Gelbard and Seinfeld, 1980). Analysis for the convergence of approximation for this type of equation was reported by Ackleh et al. (1994). The semidiscrete formulation of

equation (2.7) is

$$\begin{aligned}\frac{\partial \rho^N(t, x)}{\partial t} &= \pi^N \frac{1}{2} \int_0^x \alpha(x-y, y) \beta(x-y, y) \rho^N(t, x-y) \rho^N(t, y) dy \\ &- \pi^N \rho^N(t, x) \int_0^A \alpha(x, y) \beta(x, y) \rho^N(t, y) dy \\ &- \pi^N p \frac{f(x) \rho^N(t, x)}{\int_0^A f(x) \rho^N(t, x) dx + k_p} Z.\end{aligned}$$

where

$$\rho^N(t, x) = \sum_{k=1}^N \alpha_k^N(t) B_k^N(x)$$

denotes the computational approximation. Here B_k^N denotes linear B-spline basis functions, and π^N is the corresponding interpolation operator. Collocation leads to a nonlinear system of ordinary differential equations for the coefficients α_k^N by evaluation at the collocation grid points x_k , $k = 1, \dots, N$. This system is then solved using the package LSODE (obtained from NETLIB).

The values of a number of the biological parameters were chosen from the literature. For example, diatoms were used as the modeled phytoplankton cells because of their importance in high nutrient, productive regions and because of their hypothesized importance in aggregate formation (Hill, 1992). The minimum cell volume of the modeled diatom was $2,000 \mu m^3$, which corresponds to a radius of $7.8 \mu m$ for a spherical cell. The initial nitrate concentration was assumed to be $40 \mu M$, typical of the eutrophic regions of the North Sea. The zooplankton uptake rate used was $p = 10^5 \text{ cells day}^{-1} \text{ zooplankton}^{-1}$ and the assimilation efficiency was $\delta = 0.6$, obtained for copepods feeding on diatoms (Raymont, 1983). The relationship $cellnumber = (\frac{dx_k}{dx_1})^{\frac{1}{0.44}}$ developed by Jackson (1989) was used to describe the

number of cells with diameter d_{x_1} within aggregate of diameter d_{x_k} . The initial distribution for all the simulations consisted of single cells only with density of 10^5 cells/L. We divided our mesh into 20 sections with $x_1 = 2v_{min}$ and all the rest of the grid points were uniformly distributed with step of 0.01 mm^3 .

3. Results

The dynamics of the modeled phytoplankton blooms are a function not only of initial nutrient concentration, but of the aggregation process and of grazing as well (Fig. 5). When phytoplankton abundance is dependent only on nitrogen, nitrate is depleted after 10 days and the removal of most single cells from the upper layer via sinking takes over 300 days (Fig. 5A). When aggregate formation is included, nutrient depletion still occurs after 10 days, but removal of most particles from the surface layer occurs in approximately 240 days (Fig. 5B). The enhanced removal is due to the production of larger particles which sink more rapidly. Finally, when the grazing submodule is incorporated, the depletion of nutrients occurs after 11 days and the removal of particles takes approximately 45 days (Fig. 5C), similar to the temporal sequence found by Riebesell (1991a,b) in the North Sea.

When nutrients are non-limiting and if the temporal clearing scale of Riebesell (1991a,b) remains valid, aggregation cannot be the sole process acting to remove organic matter from the surface layer (Fig. 6). Rather, a coupling between grazing and aggregation is needed to yield the low densities observed following the bloom.

We also found that when grazers are introduced into the model under nutrient-replete conditions, oscillatory behavior of the algal-zooplankton community results (Fig. 7). These fluctuations are of a classical resource-consumer type. At the start of the simulation, the density of the zooplankton population is low. Because reproduction of new algal cells occurs throughout the duration of the simulation, grazers have abundant resources and grow until their density reaches a high level. They rapidly consume the algal population and reduce algal abundance to a relatively low level. This in turn results in a decrease in the zooplankton population density (via lower growth with a constant mortality), and the effect on the phytoplankton is reduced and the cycle is repeated. Because larger aggregates are formed from collisions of single cells, the fluctuations in the population of single-celled phytoplankton propagate through the dynamic behavior of the aggregates as well. Figs. 8A and 8B, respectively present the densities of single cells and aggregates when none of the cells in aggregates reproduce and when 25% of the cells in aggregates reproduce. In this situation with both aggregation and abundant nutrients, higher numbers of living cells in aggregates enhances removal from the surface layer.

Higher initial nitrate concentrations yield higher algal densities, which in turn leads to higher aggregate densities. Larger aggregates are formed because of higher rates of collision (Fig. 9). The dependence of the density of single-celled phytoplankton on cell radius is shown in Fig. 10. Smaller cell radii result in higher densities for the single cells in the algal population with the maximum density attained later. The coagulation process takes longer for smaller single cells and it

produces a higher density of smaller aggregates ($< 0.07 \text{ mm}^3$) because of a greater contact efficiency and higher density of single cells. The larger cells produced larger aggregates ($> 0.1 \text{ mm}^3$) at higher densities because a fewer collisions are required to form large aggregates.

The depth of the surface layer also structures phytoplankton density, with a deeper surface layer giving rise to higher densities of phytoplankton. The longer time required by aggregates to sink from a deeper surface layer plays a more important role in aggregation (Fig. 11).

4. Discussion

The interactions between marine trophic structure and aggregation processes can impact the dynamics of algal communities in the oceans. The roles of these processes in governing phytoplankton dynamics are reflected in the relative times for the removal of phytoplankton cells from the surface layer of the oceans. To compare the importance of the various processes, we assume that there is an elevated concentration of nutrients initially but minimal input through the pycnocline, a situation that often occurs during phytoplankton blooms, e.g., those of the North Atlantic Ocean (Marra and Ho, 1993). Additional nutrients increase the time for removal of algal cells from the surface layer because cells grow and reproduce when nutrients are available. Under the parameterization employed for diatoms, we find that aggregation and vertical flux cannot remove phytoplankton rapidly enough

to mimic the relevant observed time scales. In fact, in our simulations the activity of grazers is necessary in conjunction with aggregation to remove the algal population within 45 days, similar to the temporal sinking scale found by Reibesell (1991a, b) in the North Sea. The importance of this combination of processes governing marine plankton food chains also suggests that the biological processes can be more important than to the physical ones in the ocean. Our simulation results also reinforce the conclusions obtained by Jackson (1990), Jackson and Lochmann (1992), and Hill (1992) that aggregation limits phytoplankton yields and accelerates removal of senescent cells from the ocean's surface layer (Fig. 5, 6). They also corroborate the results of Jackson and Lochmann (1992) in that a higher initial nitrate concentration and a deeper mixed layer enhance aggregation (Fig. 9, Fig. 11).

Although nutrient depletion normally occurs following phytoplankton blooms, there are regions where nutrients remain non-limiting and aggregation continues (Reibesell, 1991 a,b). In these regions, the percentage of living cells in the aggregates, viewed as a function of time and cell density, is important in structuring dynamics of algal populations. Because there is a paucity of data on this parameter, future modeling efforts could be effective by using an inverse methodology to obtain an estimate for this parameter that fits the observed data. There is a distinct difference in cell aggregate densities in environments with abundant nutrients that is not present in an environment in which nutrients are depleted. We note that the density of single cells in Fig. 8A could be three times as high as

that of Fig. 8B; hence, it appears useful to estimate the number of living cells in aggregates.

Any model should be closely scrutinized for sensitive behavioral modes. In the sensitivity analysis of the model, we found that in an environment where nutrients are readily available as occurs for the setting of Reibesell (1991a,b), model output is sensitive to the power $\frac{1}{0.44}$ used in the relation $cell\ number = (\frac{dx_k}{dx_1})^{\frac{1}{0.44}}$. Hence, the validity and the universal nature of this relationship needs to be confirmed. In addition, the model output was sensitive to the power 1.17 used in the sinking velocity relation $w(R) = f_p \xi R^{1.17}$. The use of this relationship in various parts of the ocean and for all particles also needs to be confirmed. Also, we found that the model is responsive to the stickiness parameter α (Fig. 12). Because little information is available on the range of this parameter as well as its dependence on the physiology and the nutrient status of the individual cell, the sensitivity of the model to changes in stickiness emphasizes the need for investigation and estimation of this parameter. One method to obtain estimates of parameter is to use the inverse method discussed in Ackleh et al. (1994).

The representation of grazing, while of classical and current usage, can be improved. For example, a carrying capacity could be included in the formulation. We have modified the grazer component in this manner to include a carrying capacity term:

$$\frac{dZ}{dt} = p \delta \frac{\int_0^A f(x) \rho(t, x) dx}{\int_0^A f(x) \rho(t, x) dx + k_p} Z - m \frac{Z^2}{Z_c} \quad (4.1)$$

where Z_c is the zooplankton carrying capacity and the rest of the parameters are the same as in Eq.(2.6). Simulations using this equation have shown some difference in community dynamics behavior, but no difference in the importance of aggregation and grazing to phytoplankton blooms (Fig. 13). A more appropriate approach to investigate consequences of oceanographic processes on blooms is to employ a structured grazer population to investigate clearance of phytoplankton from the surface layer.

The fate of phytoplankton blooms in the ocean has been a focus of investigation for much of this century, yet we still are trying to understand the various processes which deliver organic material to the deep sea. This question is timely today in view of the questions concerning the role of the ocean in the global carbon cycle. Our modeling efforts have confirmed the importance of aggregate formation in the controls of organic matter flux from the surface, and have suggested that the interaction between grazing and aggregation is important in understanding the timing and magnitude of this flux. Future experimental work and field-based investigations, in concert with models of the relevant processes, are needed to accurately assess the role of aggregation to marine phytoplankton dynamics.

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Appendix: Figures and Tables

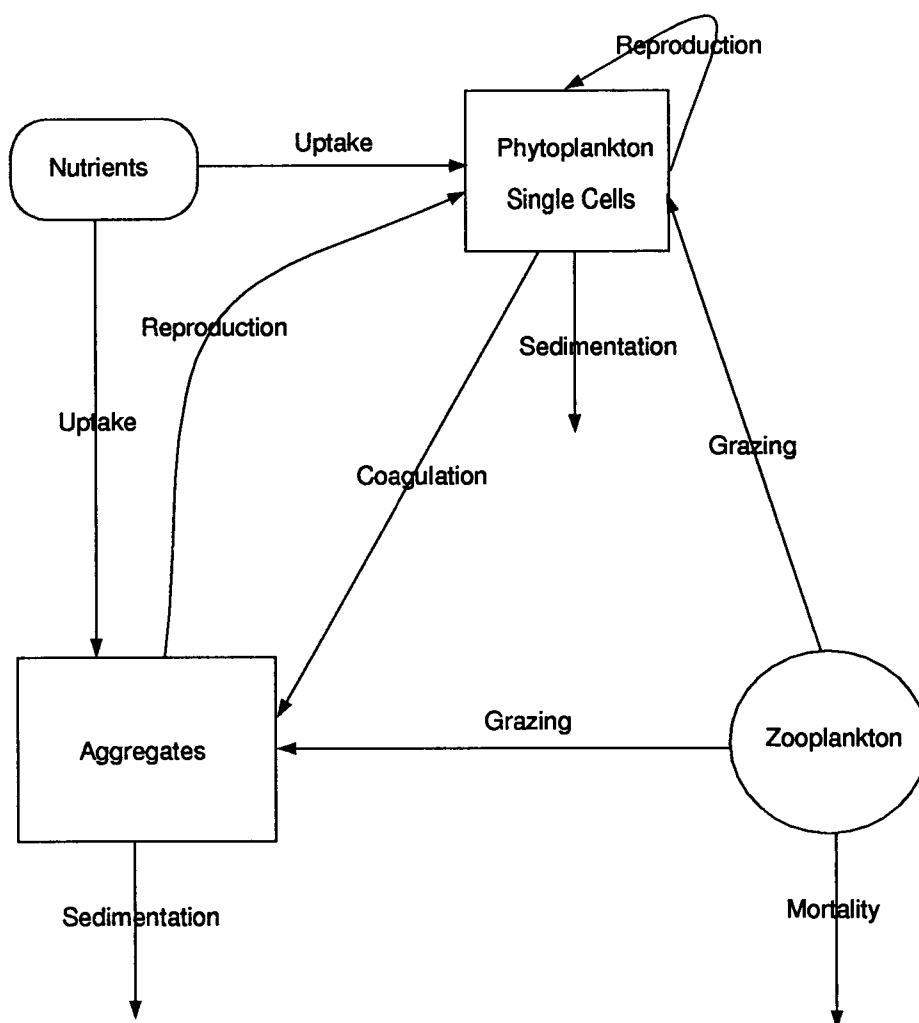
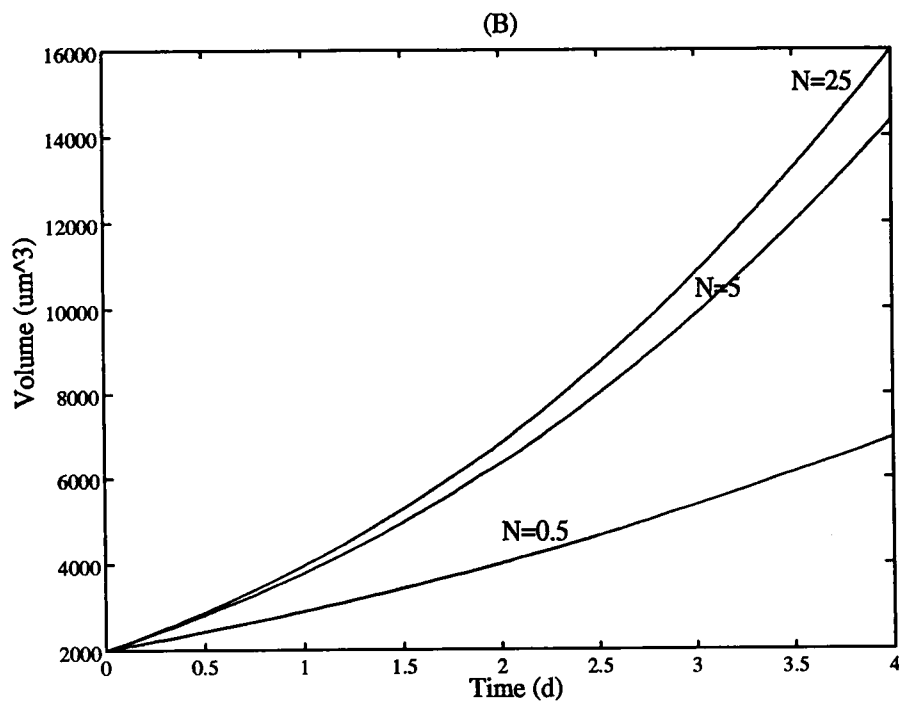
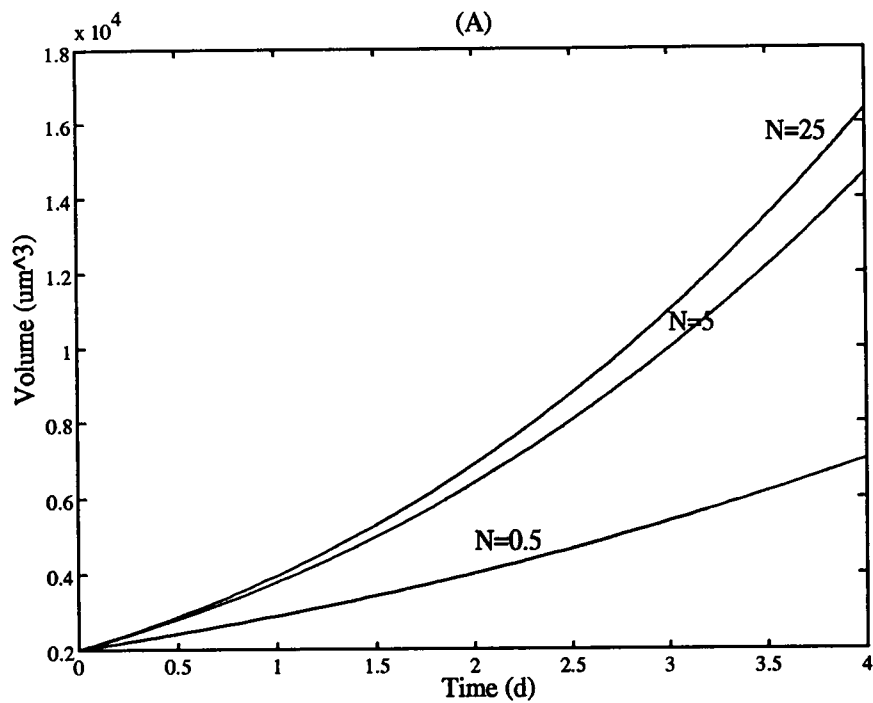


Fig. 1. Conceptual representation of the biological interactions in the algal-grazer community.



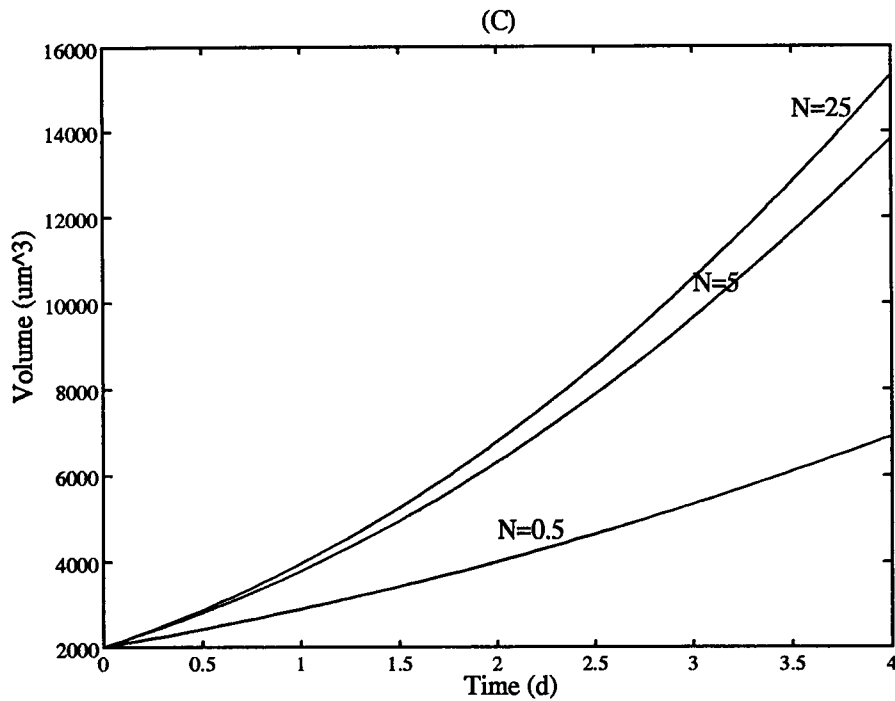


Fig. 2. The change of volume of a single cell with respect to time. The maintenance requirement b is set equal to A) 0.0084 d^{-1} B) 0.04 d^{-1} and C) 0.1 d^{-1} . Three different nutrient levels are used: (25, 5, $0.5 \mu\text{M}$).

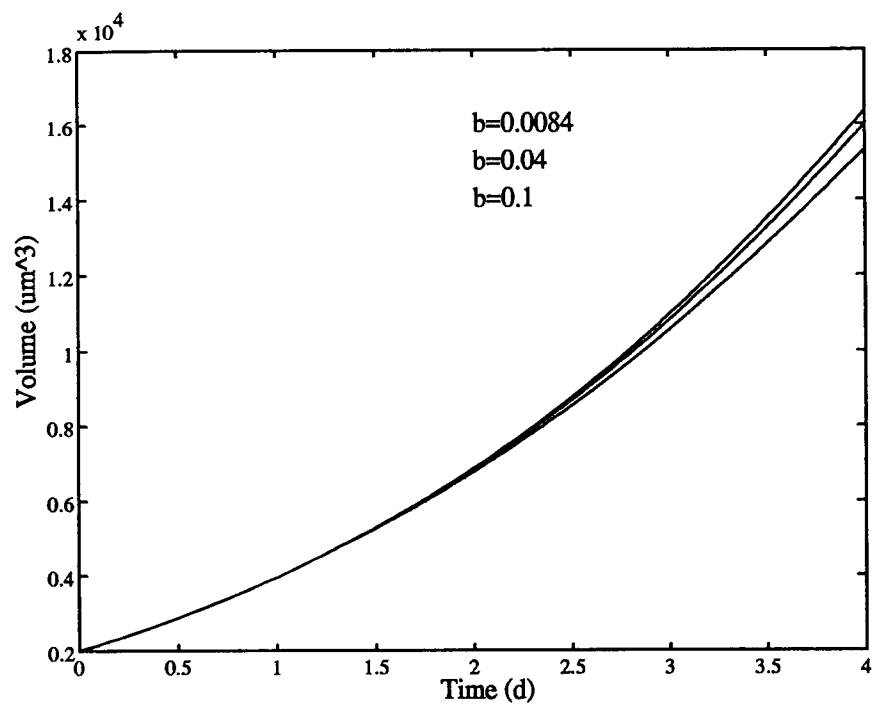


Fig. 3. The change of volume of a single cell with respect to time. The nutrient value N is equal to $25 \mu\text{M}$. Three different maintenance requirements are used: ($.0084, .04, 0.1 d^{-1}$).

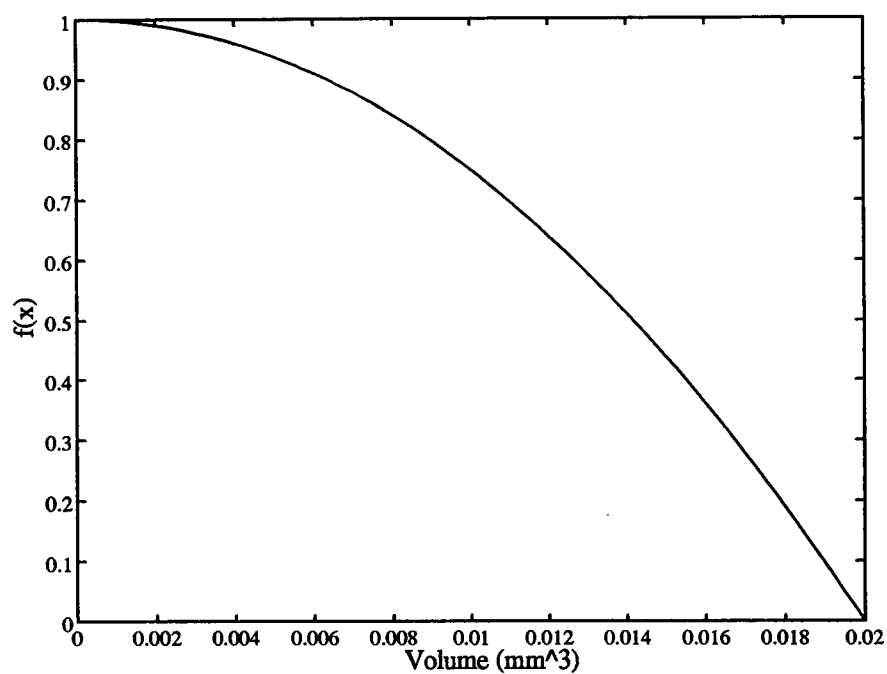
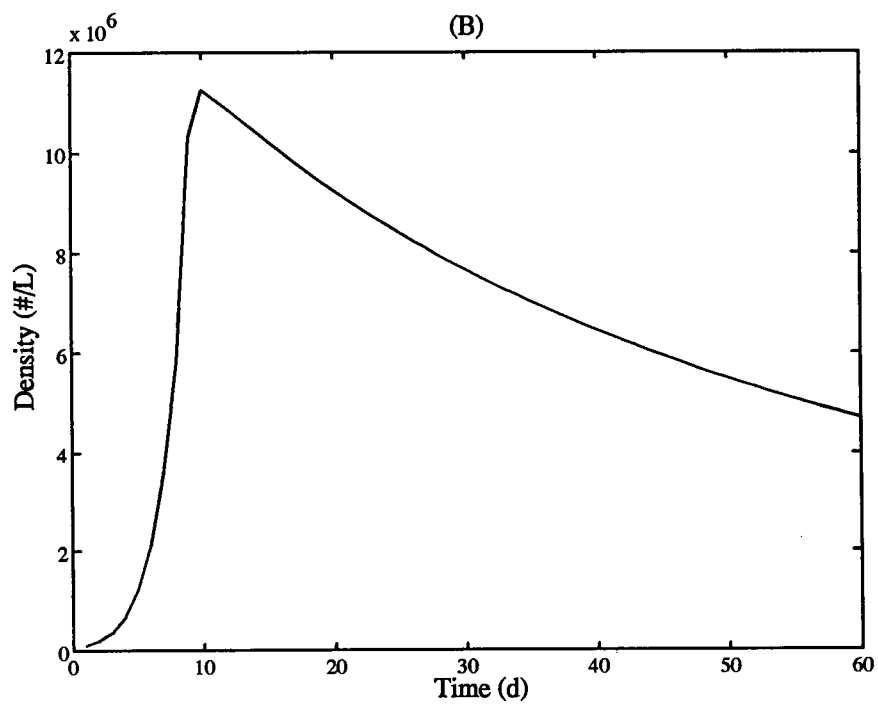
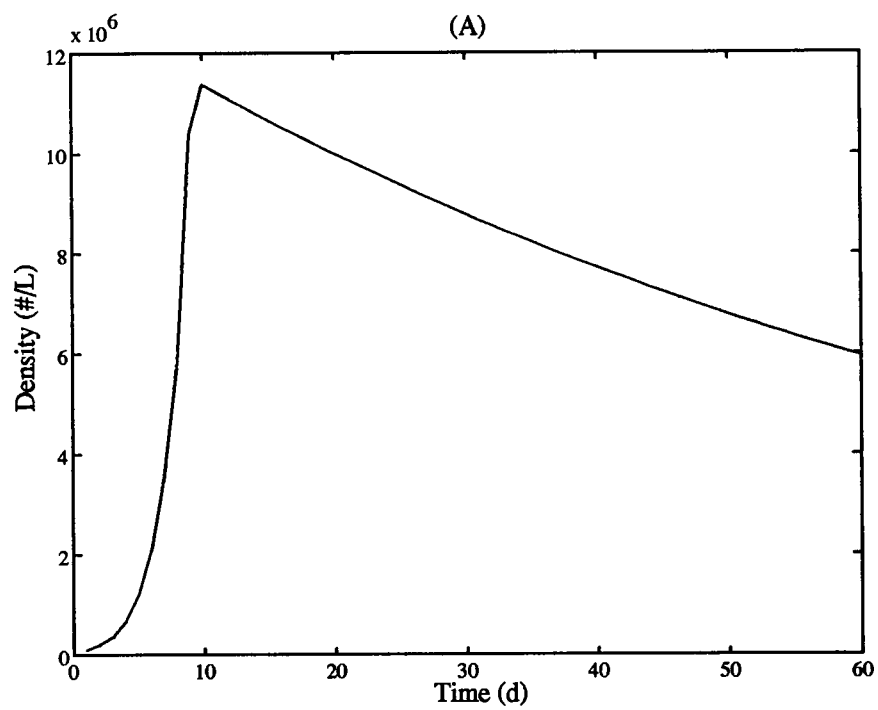
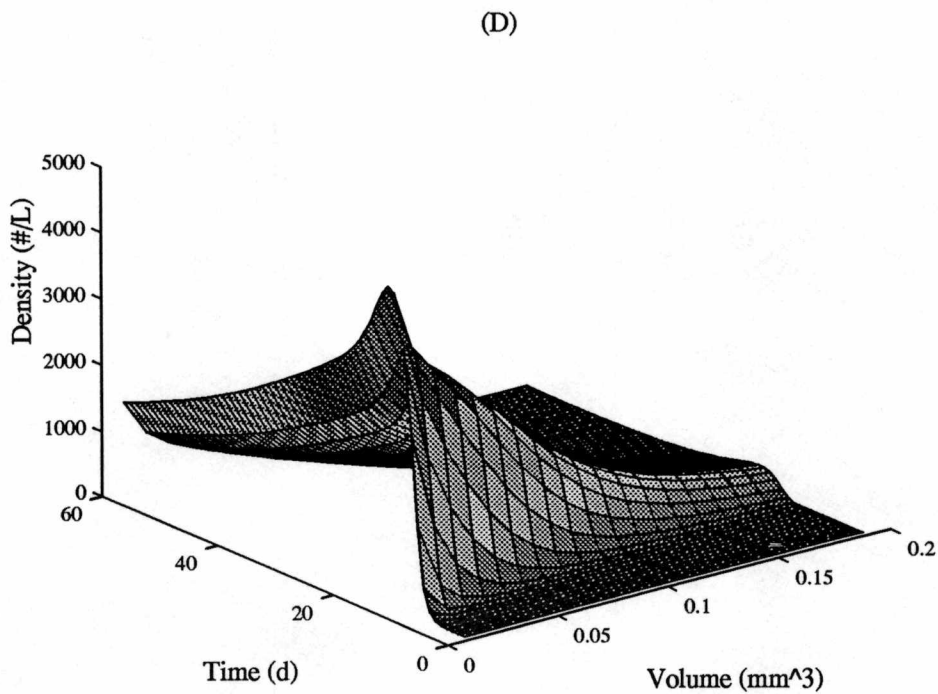
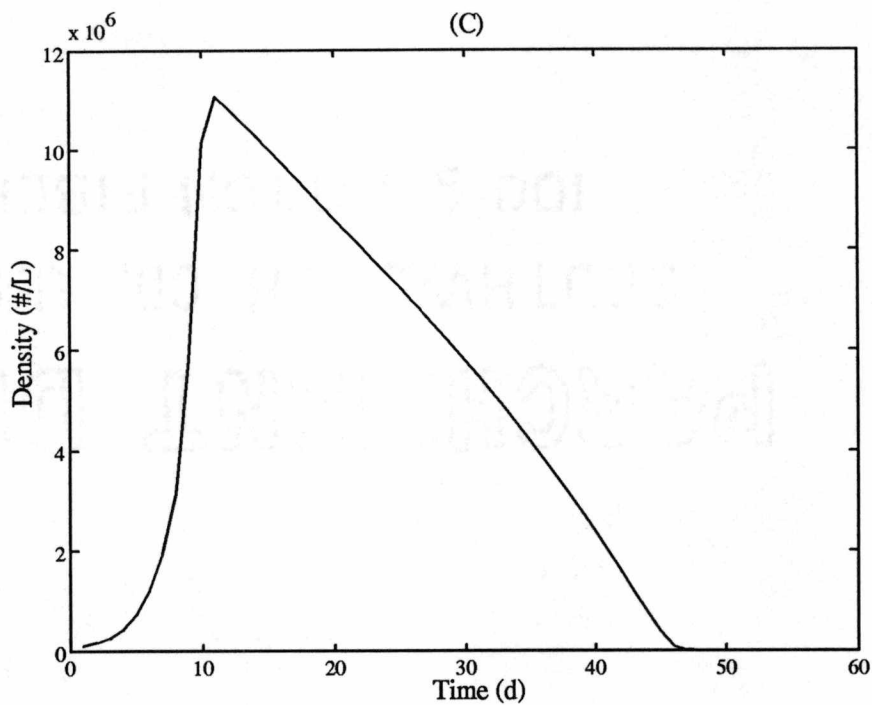


Fig. 4. The probability $f(x)$ of a zooplankter ingesting an aggregate of size x when $x_{max} = 0.02 \text{ mm}^3$.





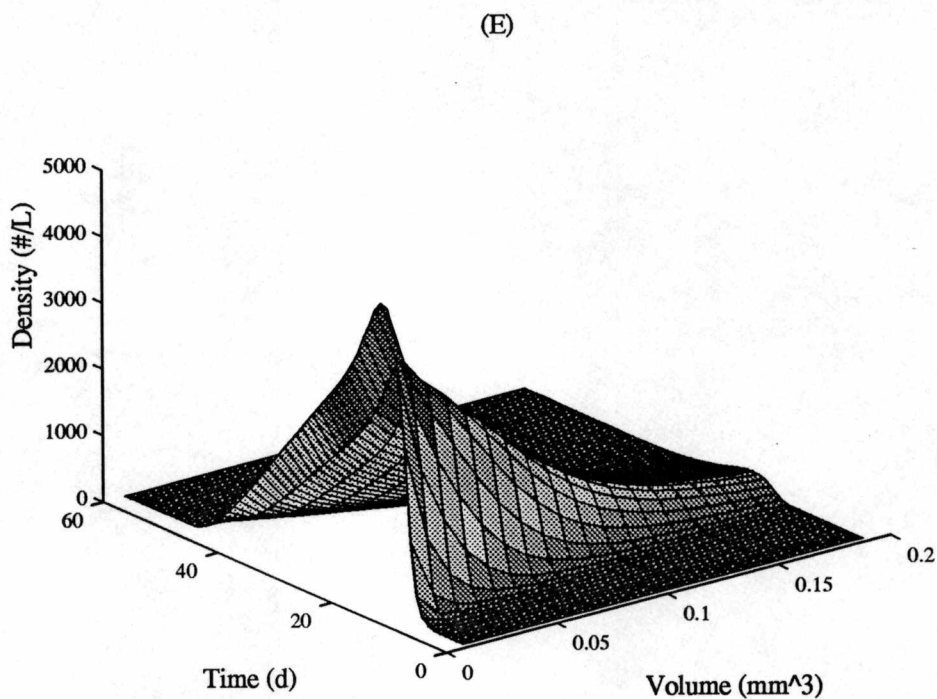


Fig. 5. The simulated response of the phytoplankton population dynamics. The initial concentration of nitrate (N_0) is $40 \mu\text{M}$ and the initial volume of single cells ($v_{\min}$) is $2000 \mu\text{m}^3$. A) The density for phytoplankton single cells when there is only nutrient limitation. The maximum density is reached after 10 days, corresponding to the time when nutrients are completely depleted. B) The analogue of (A) except that the aggregation process has been added. C) The same as (B) except that algal - grazer interactions have been added. D) The aggregate densities under the conditions described by B). E) The aggregate densities for the setting of C).

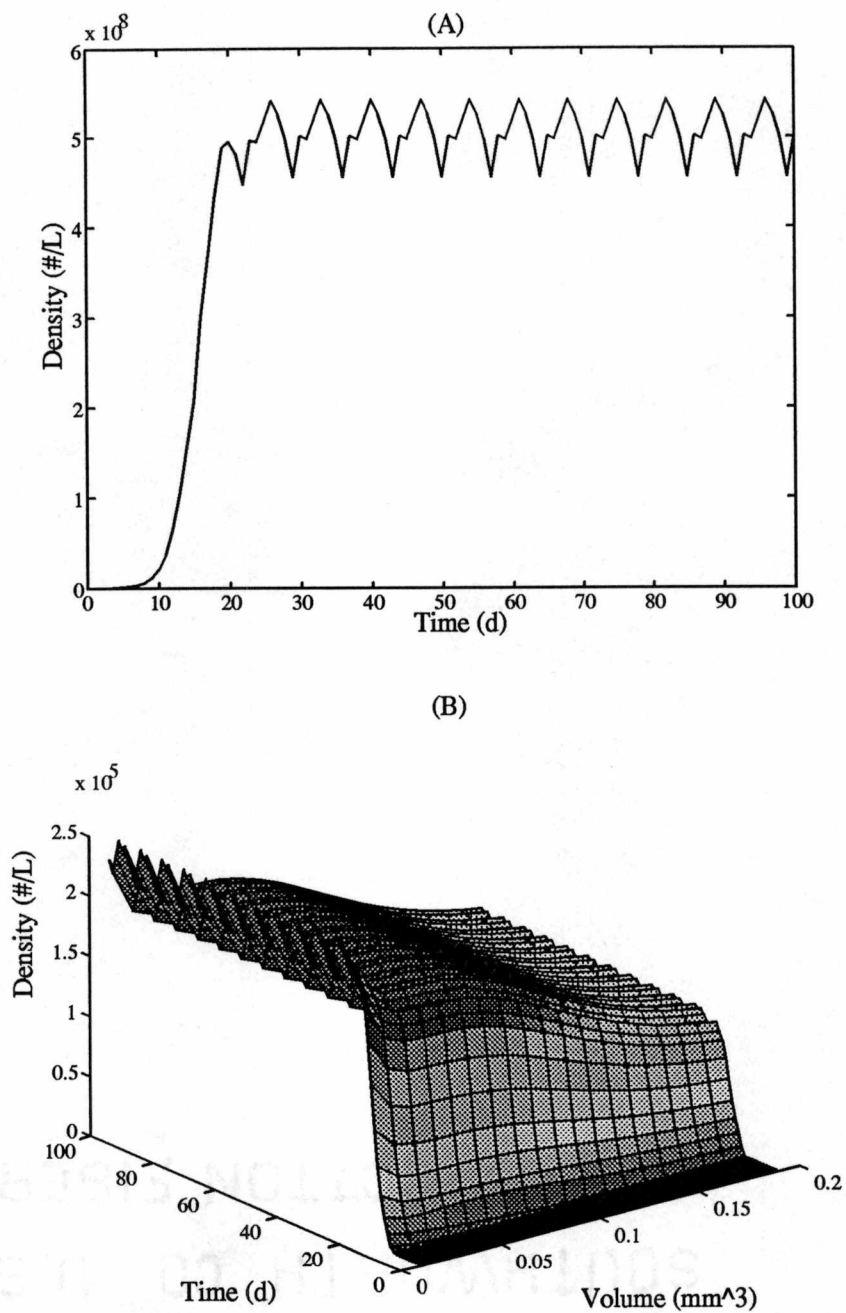
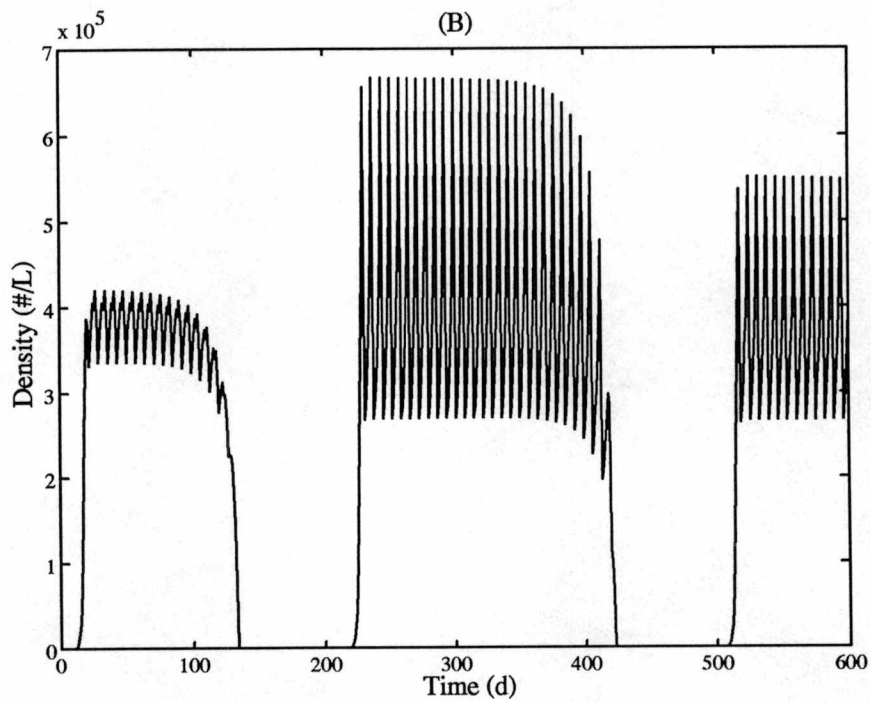
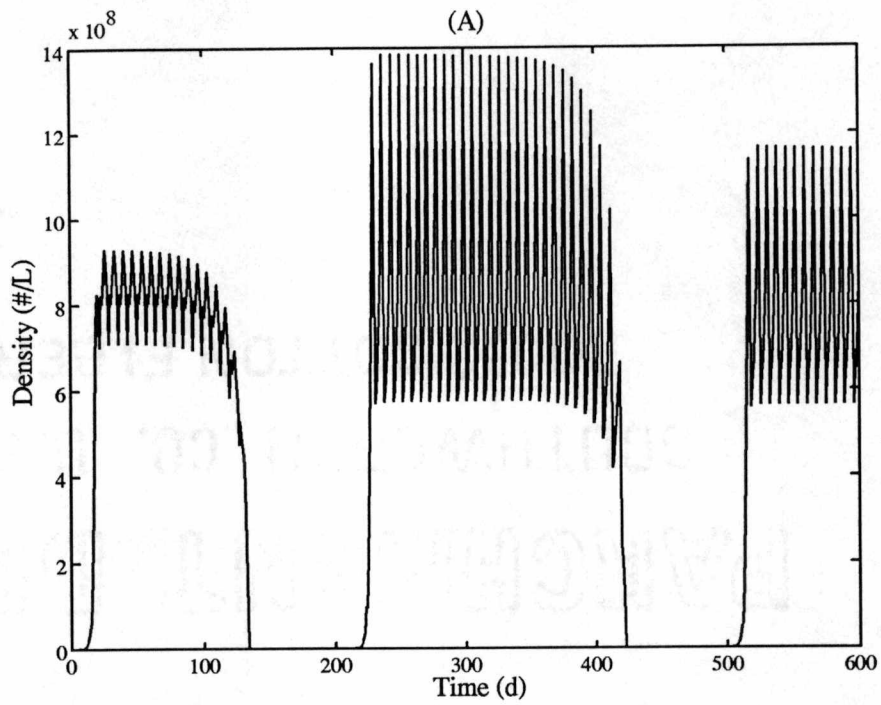


Fig. 6. The simulated response of the phytoplankton population development. A) Density of single-celled phytoplankton as a function of time B) the density of the aggregates as a function of time. The model includes aggregation, but not grazing, and nutrients are non-limiting throughout.



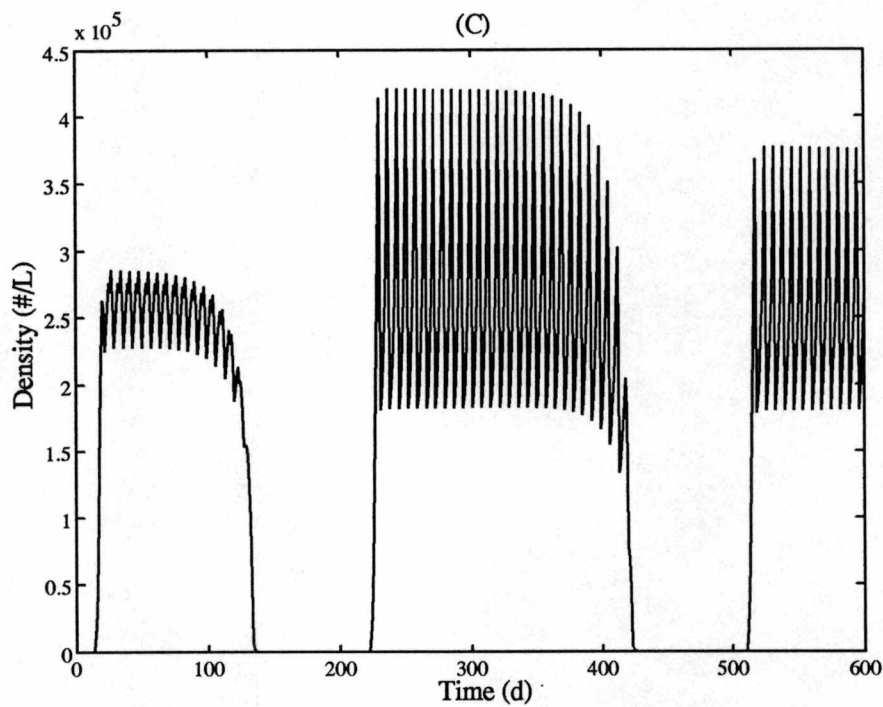


Fig. 7. Long term oscillatory behavior of the phytoplankton population. The changes in the density of A) single-cells B) aggregates of size $x_2 = 0.01 \text{ mm}^3$ and C) aggregates of size $x_{11} = 0.1 \text{ mm}^3$ with respect to time. Similar fluctuations can be observed in all other aggregate sizes. In this simulation 10% of the cells in the aggregates divided.

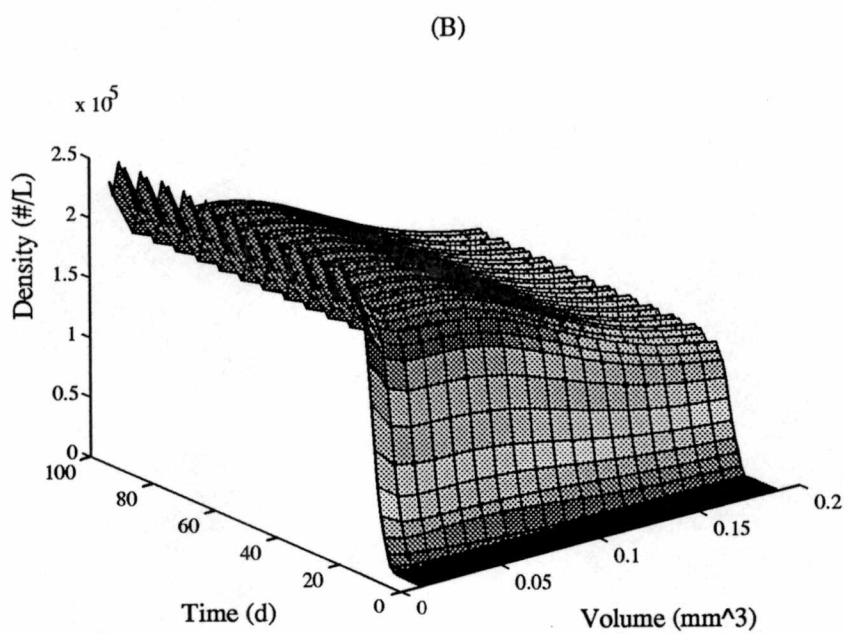
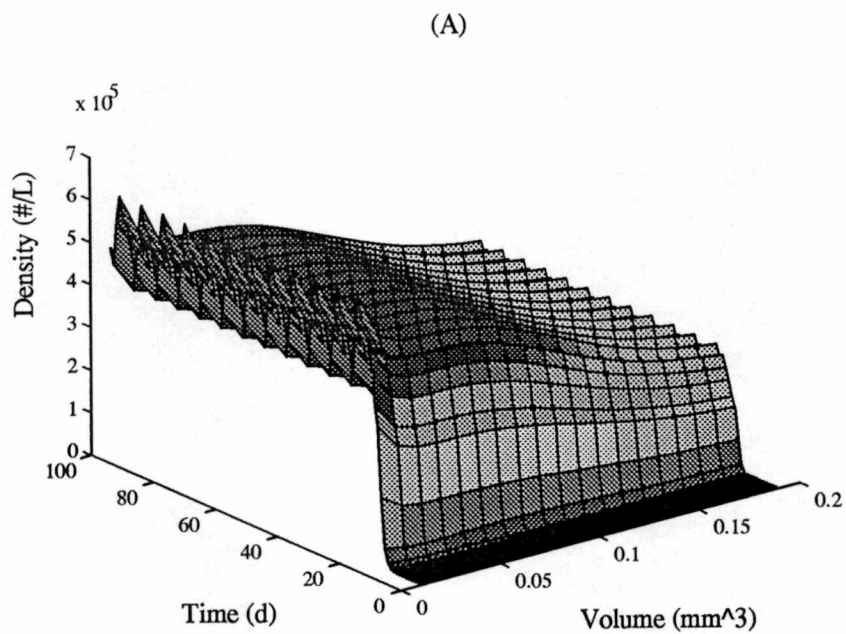
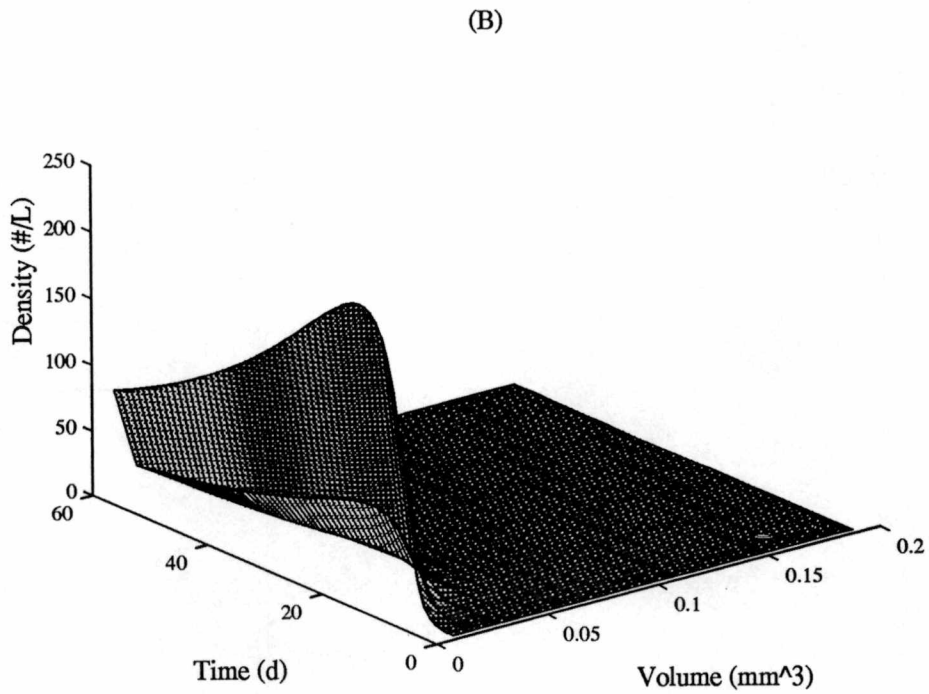
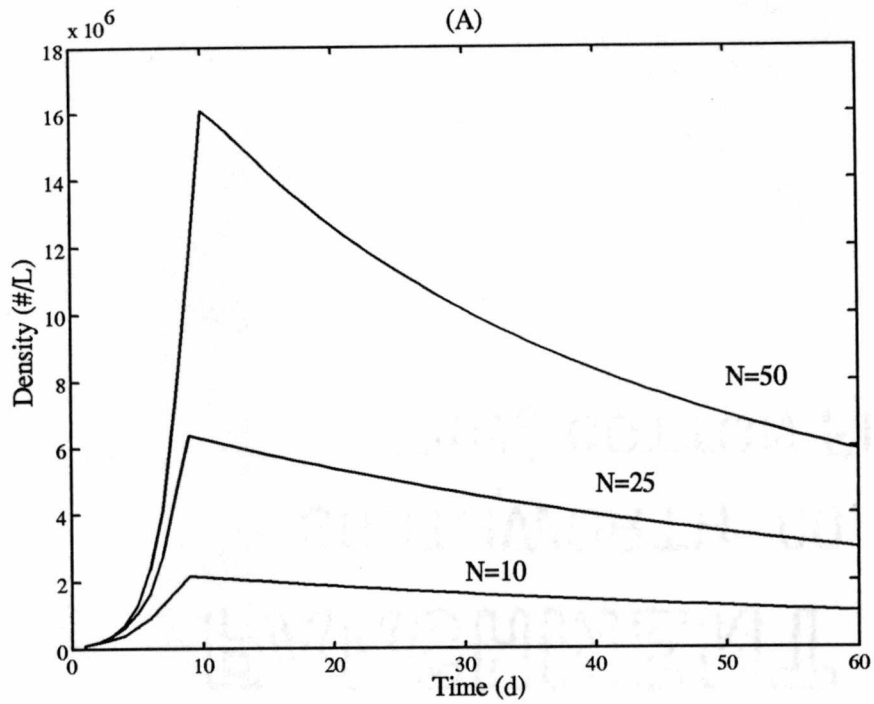
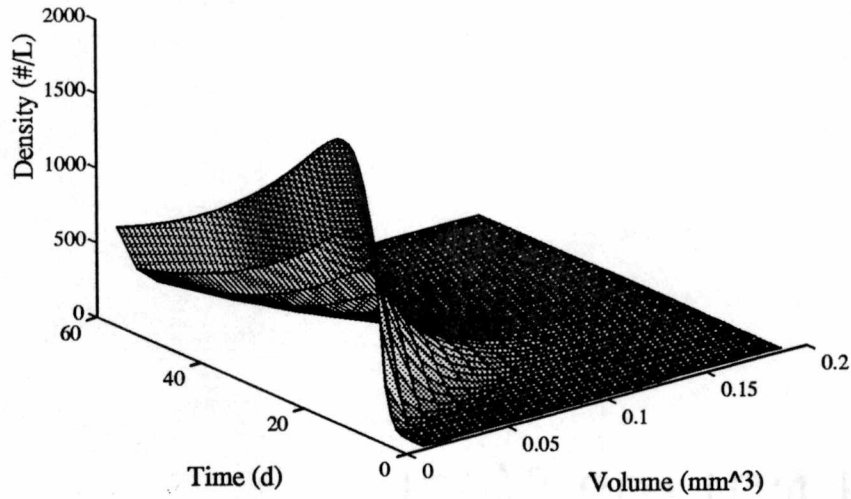


Fig. 8. The effects of cell division on aggregates density. Nutrients are not limiting in this simulation. A) 25% of the cells in aggregates divide and B) none of the cells in aggregates divide.



(C)



(D)

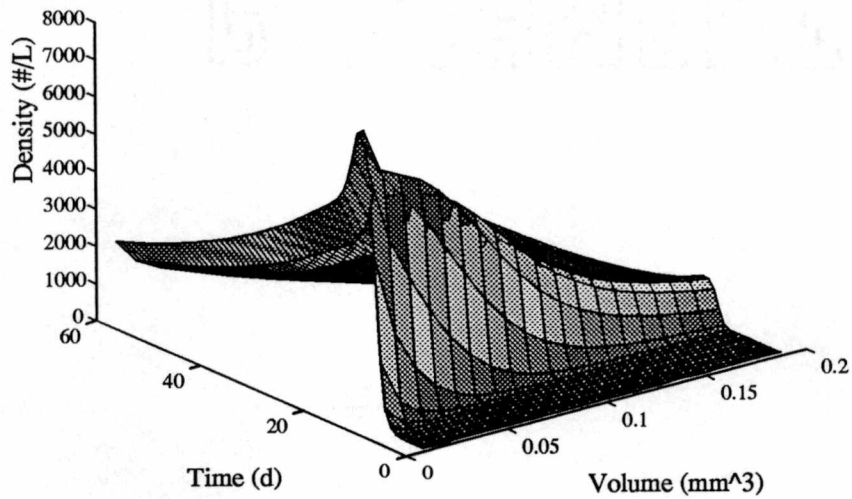
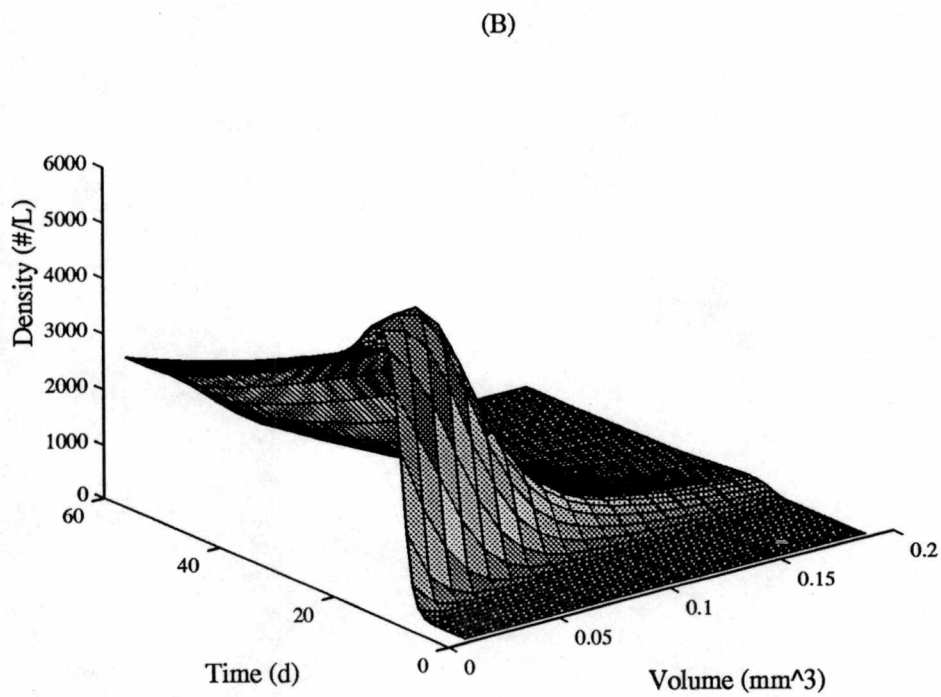
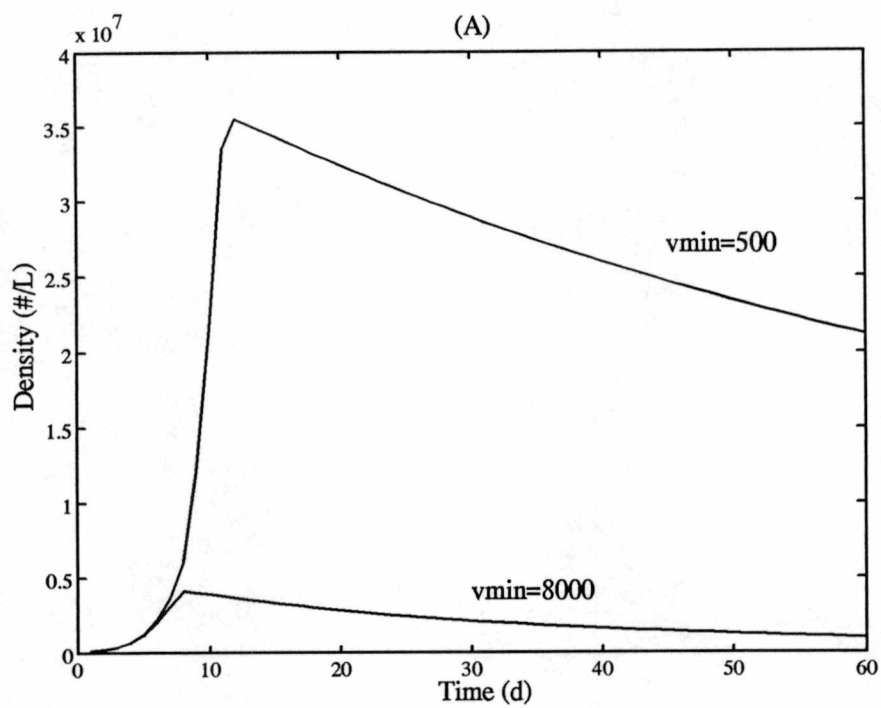


Fig. 9. The effect of nutrient concentration on the phytoplankton population. A) The density of single cells with different initial nitrate concentrations $N_0 = 10 \mu\text{M}$, $N_0 = 25 \mu\text{M}$ and $N_0 = 50 \mu\text{M}$. B) The density of aggregates with initial nitrate concentration $N_0 = 10 \mu\text{M}$. C) The density of aggregates with initial nitrate concentration $N_0 = 25 \mu\text{M}$. D) The density of aggregates with initial nitrate concentration $N_0 = 50 \mu\text{M}$.



(C)

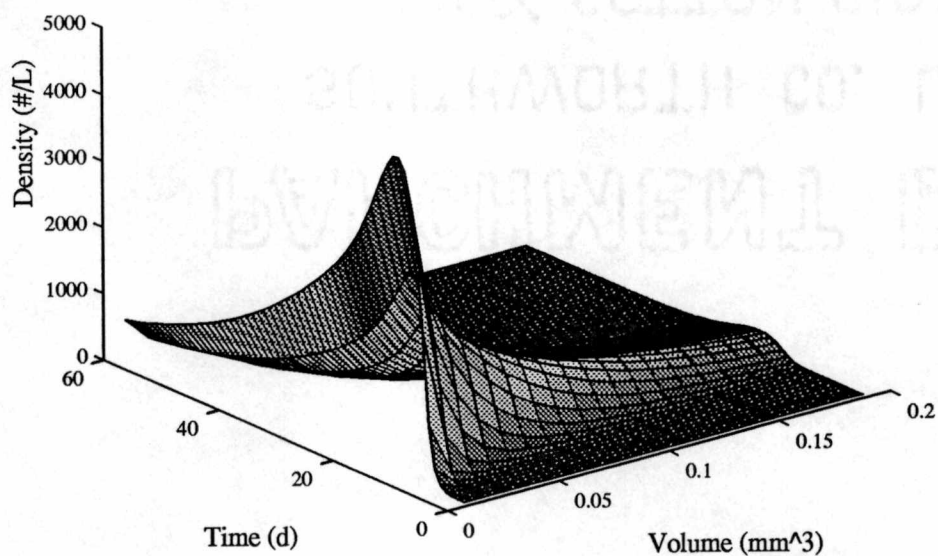
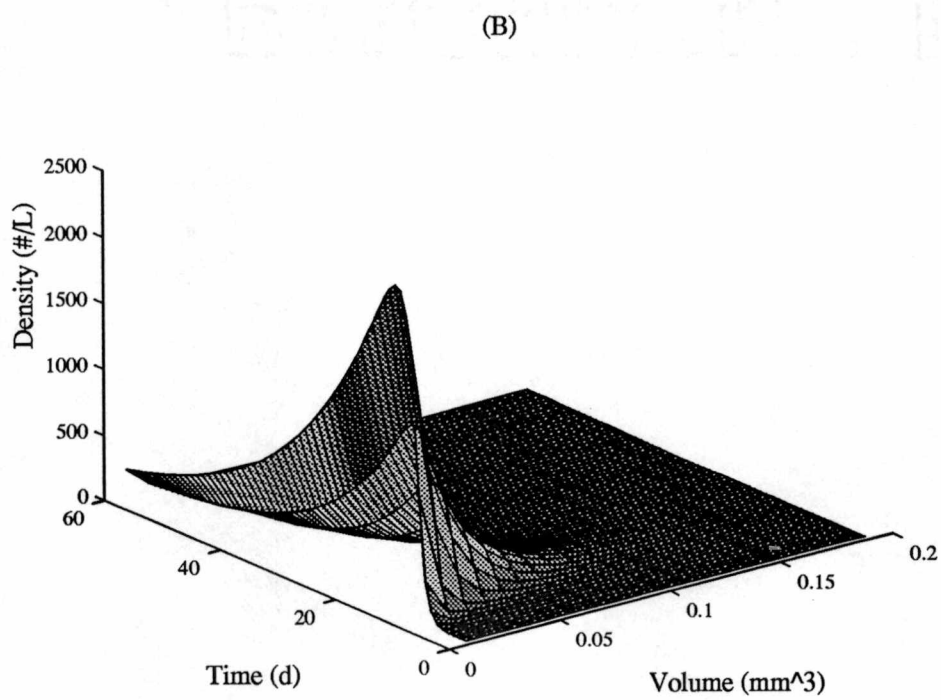
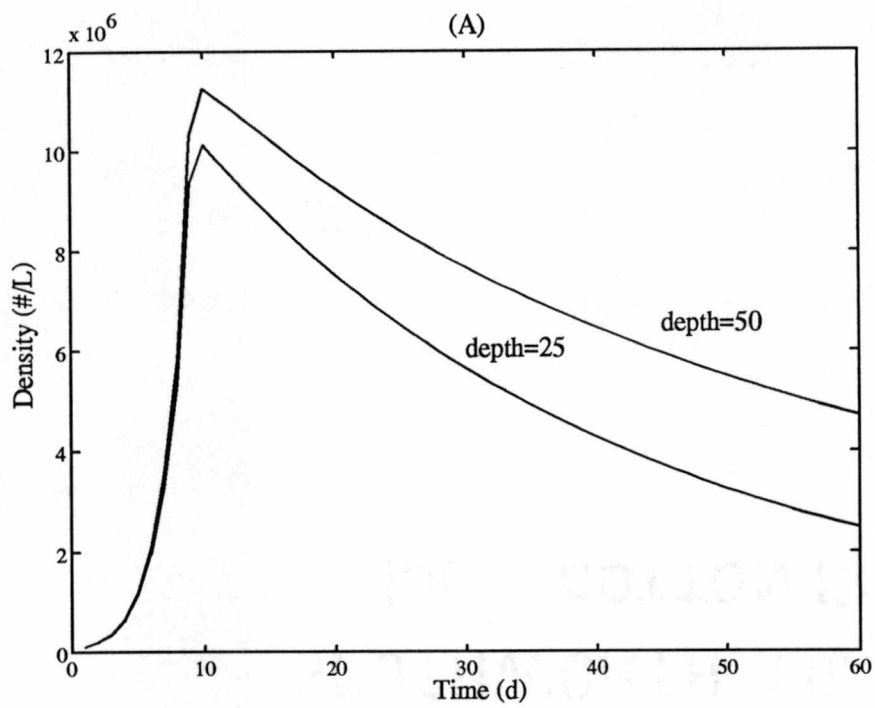


Fig. 10. The effect of the cell size on the phytoplankton dynamics. The changes in density of A) single cell when $v_{min} = 500 \mu m^3$ ($r = 4.9 \mu m$) and $v_{min} = 8000 \mu m^3$ ($r = 15.6 \mu m$) B) of aggregates for $v_{min} = 500 \mu m^3$ ($r = 4.9 \mu m$) and C) of aggregates for $v_{min} = 8000 \mu m^3$ ($r = 15.6 \mu m$).



(C)

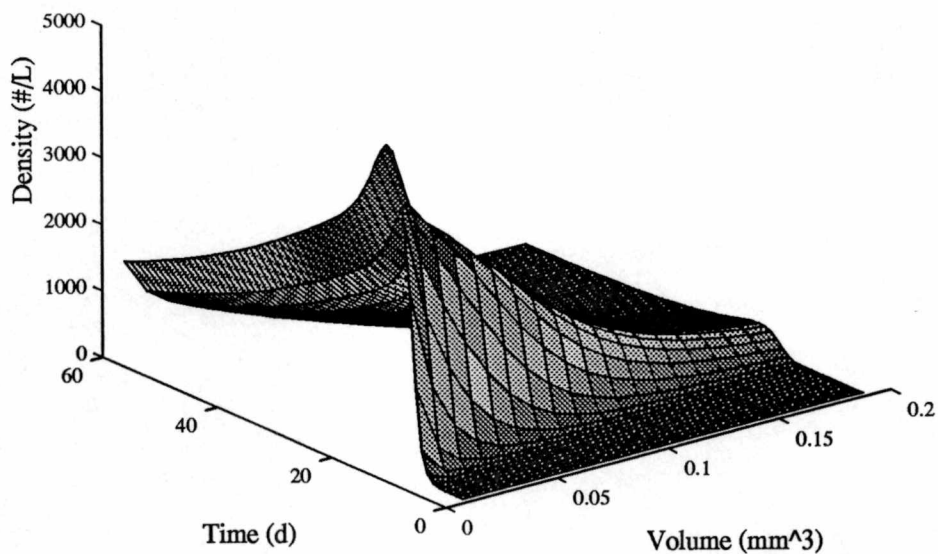
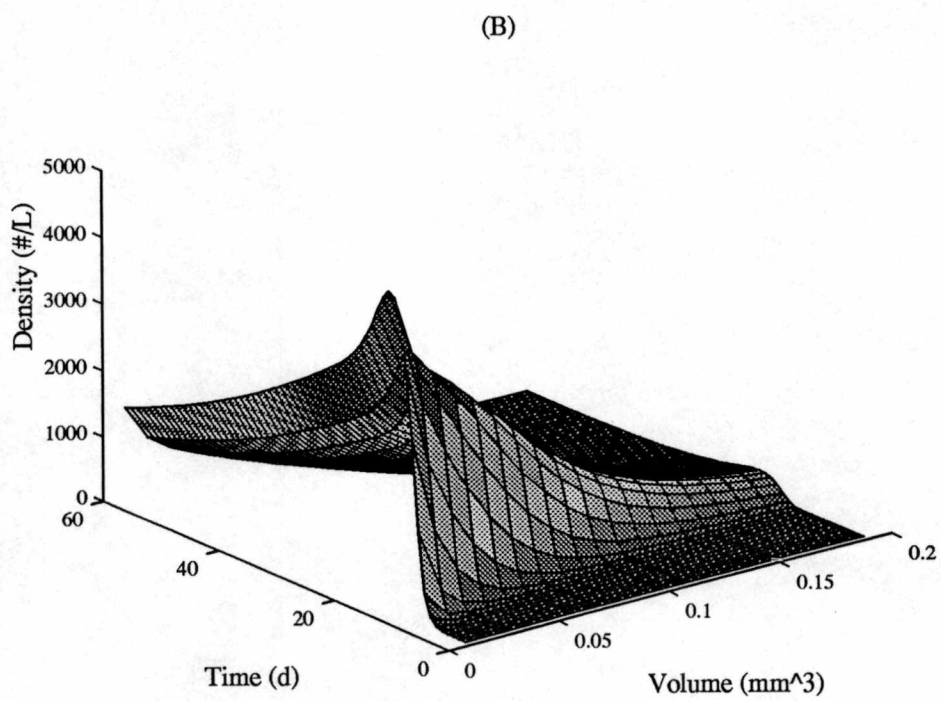
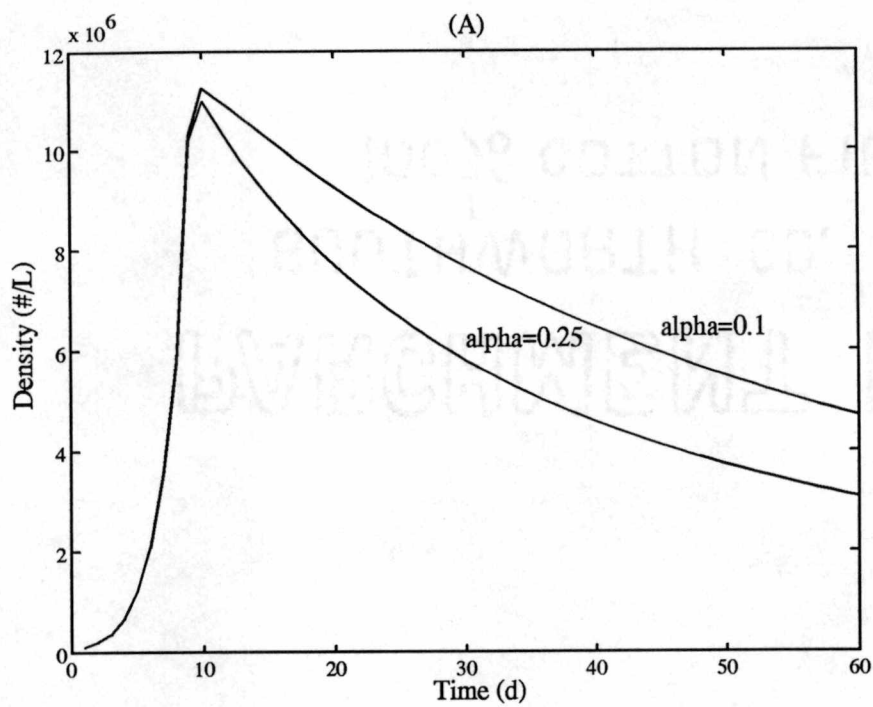


Fig. 11. The effects of the mixed layer depth on the phytoplankton dynamics. A) The density of the phytoplankton single cells when the depth of the mixed layer is equal to 25 and 50 m. B) The density of aggregates with the surface layer depth 25 m. C) The density of aggregates with the surface layer depth 50m.



(C)

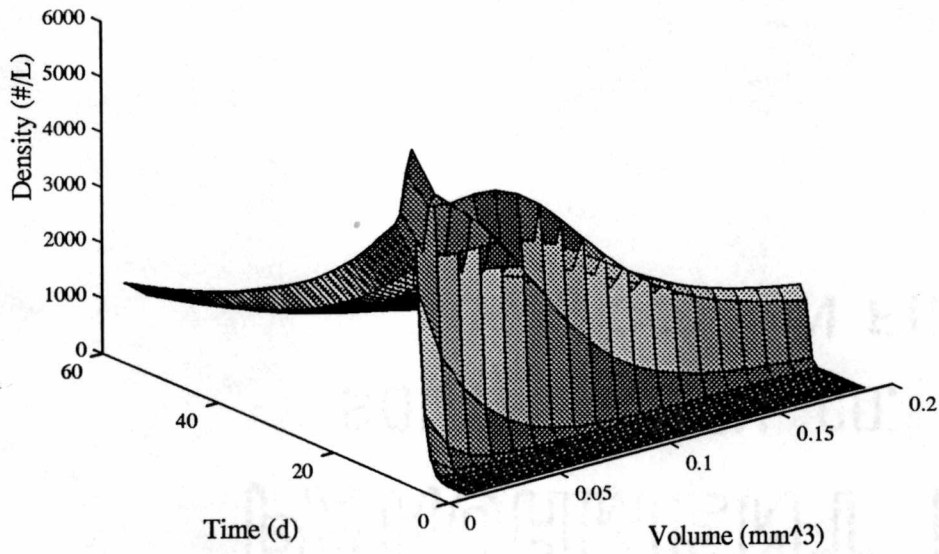
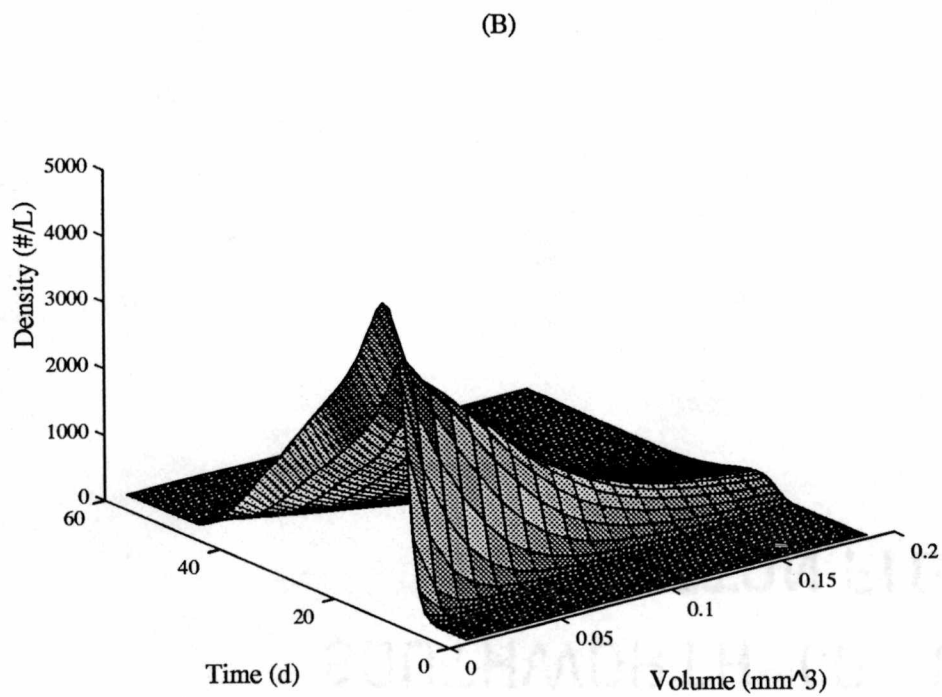
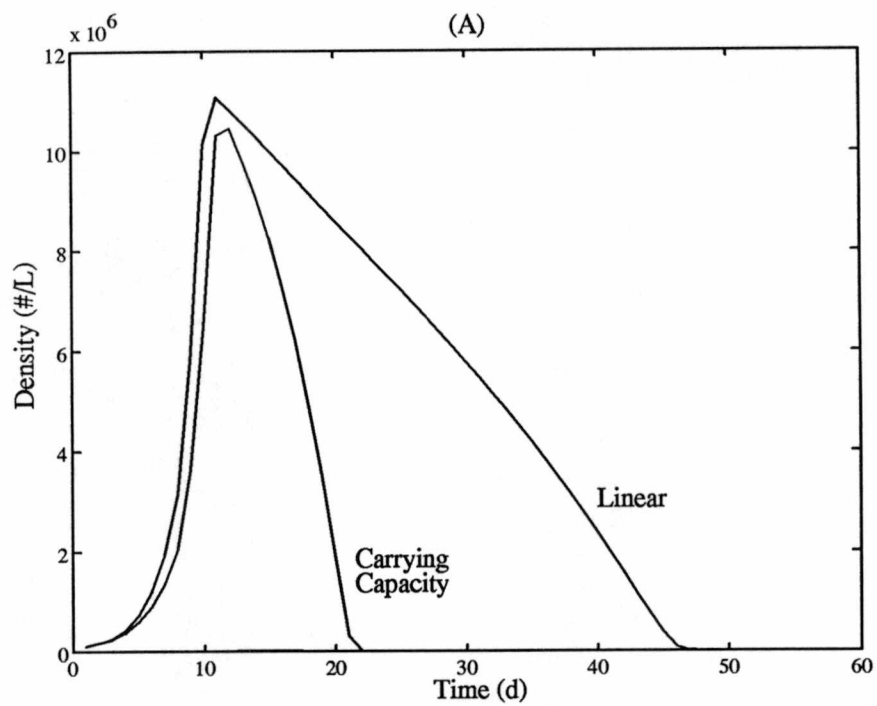


Fig. 12. The effects of the stickiness on aggregate formation. A) The single cell density for different values of α (0.1, 0.25), B) the aggregate density when $\alpha = 0.1$, and C) The aggregate density when $\alpha = 0.25$.



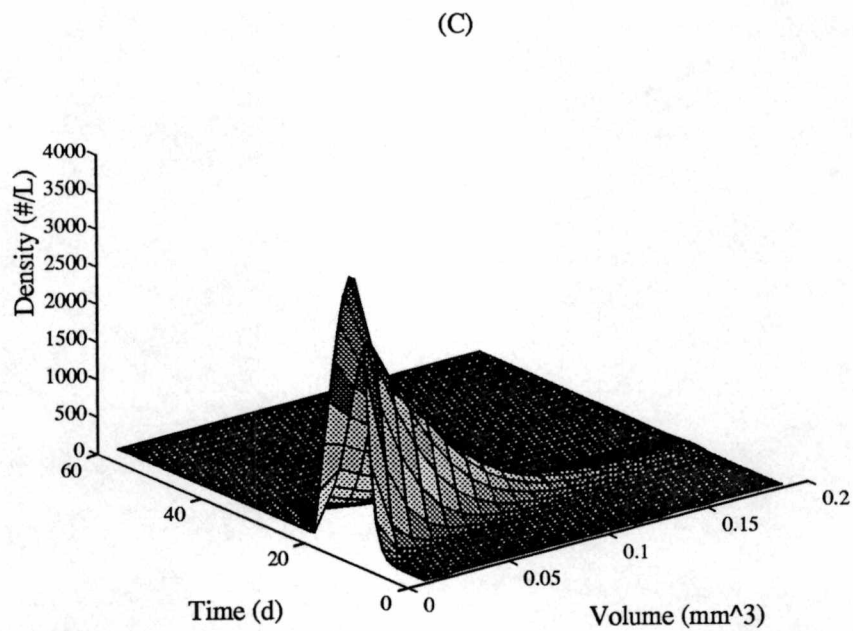


Fig. 13. The effects of inclusion of a carrying capacity on phytoplankton. A) The density of single cells using both grazing models. B) The density of aggregates using the linear grazer model. C) The density of aggregates using the carrying capacity grazer model.

Table 1.			
Parameter values and units used in the model.			
Symbol	Interpretation	value (unit)	Source
v	volume of cell	2000 – 4000 (μm^3)	Scheffer 1991 Jackson and Lochmann 1992
x	volume of aggregate	mm^3	
R	radius of aggregate	mm	
t	time	(d)	
N	Nitrate concentration	(μM)	
N_0	initial nitrate concentration	40 (μM)	
k_N	half saturation	0.5 (μM)	
a	cell growth rate	($\mu m d^{-1}$)	
b	cell maintenance rate	0.0084 (d^{-1})	
v_{min}	initial volume of cell	2000 (μm^3)	
$\rho(t, x)$	density of aggregates	($\frac{\#}{L}$)	model output
$\alpha(x, y)$	sticking probability	0.1 (nondim)	
D	surface depth	25-50 (m)	output of model
Z	density of zooplankton	($\frac{\#}{L}$)	
p	zooplankton ingestion rate	10^5 cells/d/zooplankter	Raymont 1983
δ	zooplankton assimilation efficiency	0.6 (nondim)	Raymont 1983
m	zooplankton mortality rate	0.175 (d^{-1})	Scheffer 1991

Continuation of Table 1.			
Parameter values and units used in model.			
Symbol	Interpretation	value & unit	Source
$f(x)$	grazing probability	$\begin{cases} 1 - (\frac{x-x_1}{x_{max}-x_1})^2 & x \leq x_{max} \\ 0 & x > x_{max} \end{cases}$	
x_{max}	maximum aggregate size ingested by zooplankton	(300 μm in diameter) $\approx 0.02 \text{ mm}^3$	Lancelot et al. 1991 Raymont 1983
k_p	algae half saturation constant for feeding	(25-50 ($\frac{mg C}{m^3}$)) $\approx 6 \times 10^4 - 1.4 \times 10^5 (\frac{\#}{L})$	Steele and Henderson 1981 Frost 1987
ξ	curve fit for w parameter	$1.24 \frac{1}{cm^{0.17} s}$	Jackson and Lochmann 1992
c	constant for algal carbon content	$1.67 \times 10^5 \frac{nmol}{cm^{2.28} cell}$	Mullin 1966
f_p	fall velocity scale parameter	2	Jackson and Lochmann 1992
r	radius of cell	7.8-10 μm	
m_0	Nitrogen Mass per cell	$nmol N cell^{-1}$	Mullin 1966

Part IV

WORK IN PROGRESS ON ESTIMATION OF PARAMETERS IN THE AGGREGATION PROCESS

Abstract - Aggregate formation, the genesis of larger particles from the collisions of smaller ones, is fundamental to many biological processes in the ocean. Because large particles generally sink faster than small ones, aggregate formation can be important in increasing mean particle size and accelerating the flux of biogenic matter from the ocean's surface to the deep sea. It also may limit phytoplankton population size by increasing loss rates over monthly and seasonal time scales. The formation rate of phytoplankton aggregates depends on the rate at which single cells collide and on the probability of adhesion upon collision (coagulation efficiency and sticking). Because of the lack of available data on the range of this parameter and its dependence on the size of the colliding cells, inverse methodology seems appropriate to estimate the "stickiness" parameter. Initial results described here show a good fit for the middle aggregate sizes and a reasonable fit for the small and the large ones in the least square sense.

1. Introduction

Aggregates in the ocean are composed of a variety of biologically derived organic materials, including algal cells, fecal pellets, and animal feeding structures, such as

mucus nets from pteropods and larvacean feeding structures (Alldredge and Silver, 1988). Relatively large aggregates are often observed in the ocean. For example, aggregates more than 1 mm in length are frequently observed in the ocean after algal blooms (Trent et al., 1978; Alldredge and Gotschalk, 1988a,b; Kiorboe et al., 1990). A number of models have suggested that the aggregation process can be very important in controlling the phytoplankton population by increasing their loss rate via faster sinking out of the surface layer (Jackson 1990; Hill 1992), and recent studies in the North Sea corroborate the suggestion that coagulation is an important process for determining the fate of organic matter produced by phytoplankton blooms (Riebesell 1991 a,b).

An important factor in the aggregation process is the concept of "stickiness": when two particles collide, there is some chance they will stick together to form larger particles. Laboratory studies (Kiorboe et al., 1990) and field experiments (Alldredge et al., preliminary report) have shown that algal cells have a positive probability to coagulate when they collide. However, the principal factors governing stickiness remain unclear. Kiorboe et al. (1990) have suggested that there is a relation between nutrient concentration in the medium and aggregation of phytoplankton cells. Their experiments showed that stickiness increases when nutrients are depleted from the medium. However, recent experiments by Alldredge et al. (1993) have suggested that there is only a weak relationship between nutrient concentration of the medium and the probability of one cell's sticking to another.

This work focuses on estimation of the "stickiness parameter" using the inverse

method developed by Ackleh et al. (1994) and the model presented in Ackleh et al. (1994) with a modification that includes density dependent self shading effect on the growth of phytoplankton single cell.

2. Model Review

The food-chain representation consists of a model of an individual algal cell, a coagulation model describing the aggregation process, a representation of nutrient dynamics and a grazer model. The individual model components are described below.

2.1. Individual cell model

If v is the volume of a single diatom cell, then the rate of volume change with respect to time is assumed to be the uptake rate minus the maintenance rate. Both physiological processes depend on the availability of the nutrient and the self shading effect. Cell volume growth is assumed to be proportional to surface area with the constant of proportionality a ($\mu\text{m d}^{-1}$). The maintenance costs or respiration rate is assumed proportional to the cell volume with constant of proportionality b (d^{-1}). The self shading factor s is assumed to be 1 if the density of the algal population is below a threshold ρ_{min} when no shading effects are present. It is equal to zero if the density of the algal population is above the

threshold ρ_{max} where growth is completely shut down because of shading effects.

The shading factor employed in the individual algal cell model is

$$s(\rho) = -\frac{1}{(\rho_{max} - \rho_{min})^2}(\rho - \rho_{min})^2 + 1 \quad (2.1)$$

Thus we assume that

$$\frac{dv}{dt} = \begin{cases} s \frac{N-N_T}{k_N+N-N_T}(av^{\frac{2}{3}} - bv) & N > N_T \\ 0 & N \leq N_T \end{cases} \quad (2.2)$$

with the initial condition

$$v(0) = v_{min}.$$

In (2.2), N is the concentration of the limiting nutrient, N_T is the threshold level of nutrient at which cell physiological function ceases and the cell is in a "resting state" and k_N is the half saturation constant for the limiting nutrient. In the cell life history, every cell is formed with a fixed volume (v_{min}), grows according to the above model and asexually divides when its volume doubles.

The quadratic formulation is representative in that we used other circumscribing functions such as the following linear and quadratic functions:

$$s(\rho) = \frac{1}{\rho_{max} - \rho_{min}}(\rho - \rho_{max}) \quad (2.3)$$

$$s(\rho) = \frac{1}{(\rho_{max} - \rho_{min})^2}(\rho - \rho_{max})^2 \quad (2.4)$$

The results were not sensitive to the function used (Fig.1).

2.2. Grazer-Aggregate model

If $\rho(t, x)$ is the density of the aggregates with volume x at time t , then the number of aggregates in the range x and $x + dx$ is ρdx . To describe the rate of change of ρ due to coagulation we have used the equation employed by Smoluchowski (1917) to investigate the kinetics of the coagulation of colloidal solutions, by Gelbard and Sienfeld (1978) to describe the coagulation of homogeneous particles and by Jackson and Lochmann (1992) to describe the aggregation of phytoplankton cells. This equation is as follows:

$$\begin{aligned} \frac{\partial \rho(t, x)}{\partial t} = & \frac{1}{2} \int_0^x \alpha(x-y, y) \beta(x-y, y) \rho(t, x-y) \rho(t, y) dy \\ & - \rho(t, x) \int_0^A \alpha(x, y) \beta(x, y) \rho(t, y) dy = F(\rho(t, x)), \end{aligned} \quad (2.5)$$

where $\beta(x, y)$ is the coagulation kernel for collision of two particles, one with volume x and the other with volume y and $\alpha(x, y)$ is the probability that they stick after colliding (e.g, Pruppacher and Klett, 1980). The first term in (2.5) expresses the rate at which collisions occur to form new particles with volume between x and $x + dx$ while the second term expresses the rate at which collisions cause particles to be lost from that size class due to aggregation with other particles from the same interval.

The coagulation kernel $\beta(x, y)$ consists of two parts, both of which are sym-

metric and non-negative (McCave 1984, Riebesell and Gladrow, 1992). For more details see Part III of this dissertation.

If aggregates of size x sink at velocity $w(x)$, then adding particle loss due to sinking in the equation results in

$$\frac{\partial \rho(t, x)}{\partial t} = F(\rho(t, x)) - \rho(t, x) \frac{w(x)}{D}, \quad (2.6)$$

where D is the depth of the surface layer. It is assumed that if a cell sinks from the surface layer it cannot re-enter. The settling velocity of an aggregate of radius $R = (\frac{3x}{4\pi})^{\frac{1}{3}}$, is given in Eq. (2.5) of Part III in this dissertation.

To investigate the effects of grazing, we employ the generic grazing representation for the dynamics of zooplankton in Part III of this dissertation, Eq. (4.1), this model takes the following form:

$$\frac{dZ}{dt} = p \delta \frac{\int_0^A f(x) \rho(t, x) dx}{\int_0^A f(x) \rho(t, x) dx + k_p} Z - m \frac{Z^2}{Z_c}$$

Adding the loss of aggregates due to grazing to Eq. (2.6) yields

$$\frac{\partial \rho(t, x)}{\partial t} = F(\rho(t, x)) - \rho(t, x) \frac{w(x)}{D} - p \frac{f(x) \rho(t, x)}{\int_0^A f(x) \rho(t, x) dx + k_p} Z. \quad (2.7)$$

Eqs. (2.7) and (4.1) of Part III coupled with (2.2) form the aggregation, algal and zooplankton community model without nutrient dynamics. The same procedure as in Part III of this dissertation is used to compute the change of dissolved nutrient with respect to time.

2.3 Numerical procedure

To solve Eq. (2.7) we use the spline-based collocation method (Gelbard and Seinfeld, 1980; Ackleh et al. 1994). Analysis for the convergence of approximation for this type of equation was reported by Ackleh et al. (1994). For more details see Appendix I.

For estimation of the parameter α we used the inverse method discussed in Ackleh et al. (1994). This method is based on the minimization of the function

$$J^N(\alpha) = \sum_{i,j} |\rho^N(t_i, x_j; \alpha) - z_{i,j}|^2 \quad (2.8)$$

over $\alpha \in Q$, the parameter state space.

The notation $\rho^N(t_i, x_j; \alpha)$ shows the dependence of the solution of the model on the parameter α . $z_{i,j}$ are the observations found in Riebesell (1991). We have chosen the parameter state space to be of the following form:

$$Q = \{f : f(r_1, r_2) = c_1 \frac{(r_1 + r_2)^{c_3}}{(c_2 + (r_1 + r_2))^{c_3}}, 0 \leq c_1 \leq 1, c_2 \geq 0, c_3 \geq 0\} \quad (2.9)$$

where r_1 and r_2 are the radii of the colliding aggregates. This illustrates the dependence of the parameter α on the size of the colliding cells. Because the difference in magnitude of aggregate classes decreases exponentially with increasing size, Eq. (2.8) is scaled to give equal importance for the higher classes in the least

square estimate as in the following:

$$J^N(\alpha) = \sum_{i,j} |x_j(\rho^N(t_i, x_j; \alpha) - z_{i,j})|^2. \quad (2.10)$$

This relationship implies that volume density is now the variable fitted instead of number density. Details on the model and the numerical procedure are found in Ackleh et al. (1994).

3. Results

To obtain an initial estimate, we first chose $c_2 = 0$ (i.e constant α). However such a choice gave over-estimation of the first size class and under-estimation for the rest of the classes for all times. Since the first size class has diameter of 0.1-0.2 mm, setting $c_2 = 0.1$ might affect the "stickiness" probability of this class more seriously than the rest of the size classes by decreasing it, and hence might result in smaller over-estimation of the data while the higher "stickiness" probability for the rest of the classes might decrease the under-estimated data values. Then c_3 is chosen ($c_2 = 0.1, c_3 = 2$) to indicate the dependence of the "stickiness" probability on the surface area of the colliding cells. Then, the inverse method estimates c_1 yielding $c_1 = 0.889$. Fig.2 represents the difference between the model output using the α in (2.9) and the observed data found in Reibesell (1991a,b). Notice that in the first class the model always over-estimated the observed data and in the other classes there was over-estimation of the observed data close to the 19 th

day, the peak of the bloom. We have also calculated the difference between the model output and the observed data for each class in the least square sense, i.e., for aggregates in size class x_j the difference is equal to

$$\sum_{i,j} |x_j(\rho^N(t_i, x_j; \alpha) - z_{i,j})|^2$$

and found the following results: 452.9, 229.6, 276.6, 341.5, 415.8 for the first, second, third, fourth and fifth size class respectively. Smaller differences are present in the middle sizes classes than the first and the last size classes.

4. Discussion

The formation of phytoplankton aggregates by coagulation processes depends on the particle contact rate and the stickiness of the cells. While the collision rate between particles is a function of fluid dynamics, the sticking efficiency depends on a variety of physical, chemical and biological factors (Kiorboe et al. 1990). Suspended particles, including phytoplankton have a negative surface charge and, therefore, are surrounded by a cloud of positive cations, resulting in repulsive electrostatic forces that decline with the square of interparticle distance. In seawater this cloud of cations is compressed and the repulsive forces may, therefore, be offset by attractive van der Waal forces (Kiorboe et al. 1990) that are proportional to the cube of the interparticle distance. Among important biological factors, it has been suggested that elevated excretion of mucus and polysaccharides such as

that observed in nutrient depleted cells (e.g. Joiris et al. 1982) would increase phytoplankton stickiness.

There could be several reasons that the goodness of the fit was better for middle classes (Fig.2). One is that the shape of the aggregates is presently assumed spherical. Many diatom species have extruding spines or hairs that may give rise to "mechanical" sticking or entangling of particles. For instance, diatoms of the genus *Thalassiosira* have very fine chitin fibrils that radiate outward from the cell (Guillard and Ryther 1962, McLachlan et al. 1965). Extrusions may also increase the "effective" size of suspended cells, thus increasing the interparticle encounter rate. Hence, improving our model by including the shape of the cell might improve the result of the fit. Another reason might be that the coagulation kernel is overestimated for the smaller aggregates. The contact efficiency for both the shear and differential settling are underestimated for larger aggregate sizes. The power in Eq. (2.9) could be chosen higher than 2, or another form of the stickiness function such as a function that decreases exponentially with decreasing size might be used. A choice of function that depends on the nutrient availability might make a difference since it has been suggested (Kiorboe, 1990) that stickiness increases with increasing nutrient limitation. There are many important parameters in this model that require adequate estimates before arriving at reasonable model representations of oceanic aggregation. For example, one can combine both $\alpha(x, y)$ and $\beta(x, y)$ as one function and use the inverse method to estimate this product. This has the advantage of reducing the number of uncertain parameters in the model.

It has also been suggested that bacteria plays a role in bonding particles together in aggregates (e.g. Riebesell, 1991a,b; Biddanda 1985). Because bacteria always occur in natural phytoplankton aggregates (Alldredge and Silver 1988) we may be able to improve our model by including the role of bacteria in the dynamics of aggregates.

In this estimation procedure we have been able to demonstrate two important concepts. The first is that with a simple choice of α , our model can reasonably represent at least to first order approximations, the aggregation process in the ocean. The second is that an estimate can be obtained for a parameter on which little information is available by using a method that enjoyed past success (Banks and Kunisch, 1989; Banks 1985). The balance in the over-estimation of the data and the under-estimation in the least square sense in Fig.1C is another indicator that the methodology is appropriate.

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Appendix: Figures

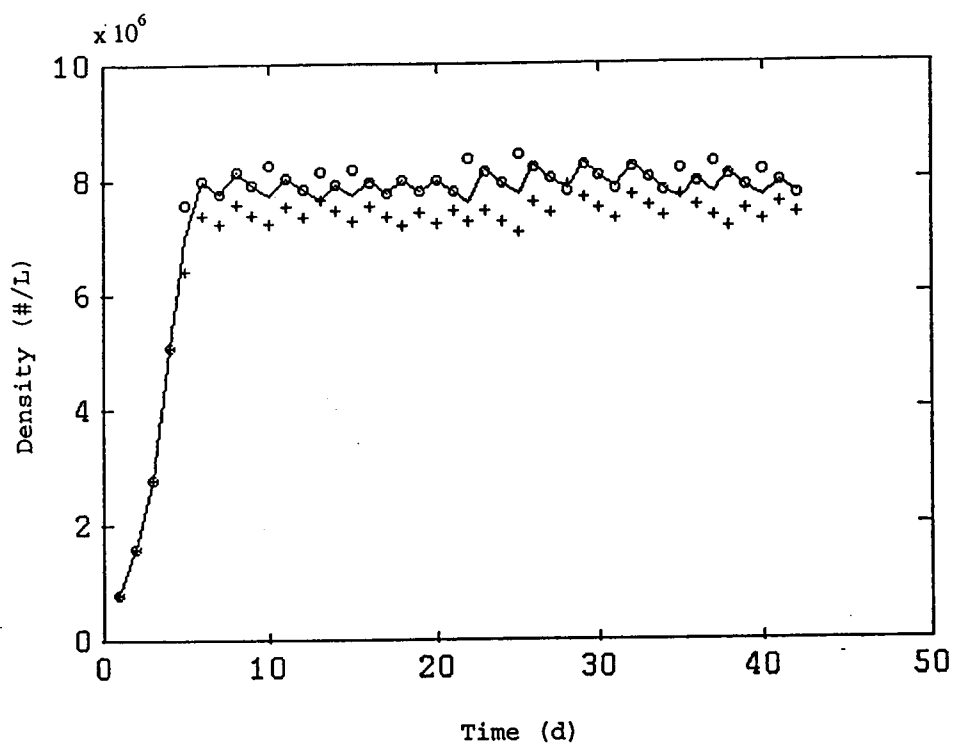
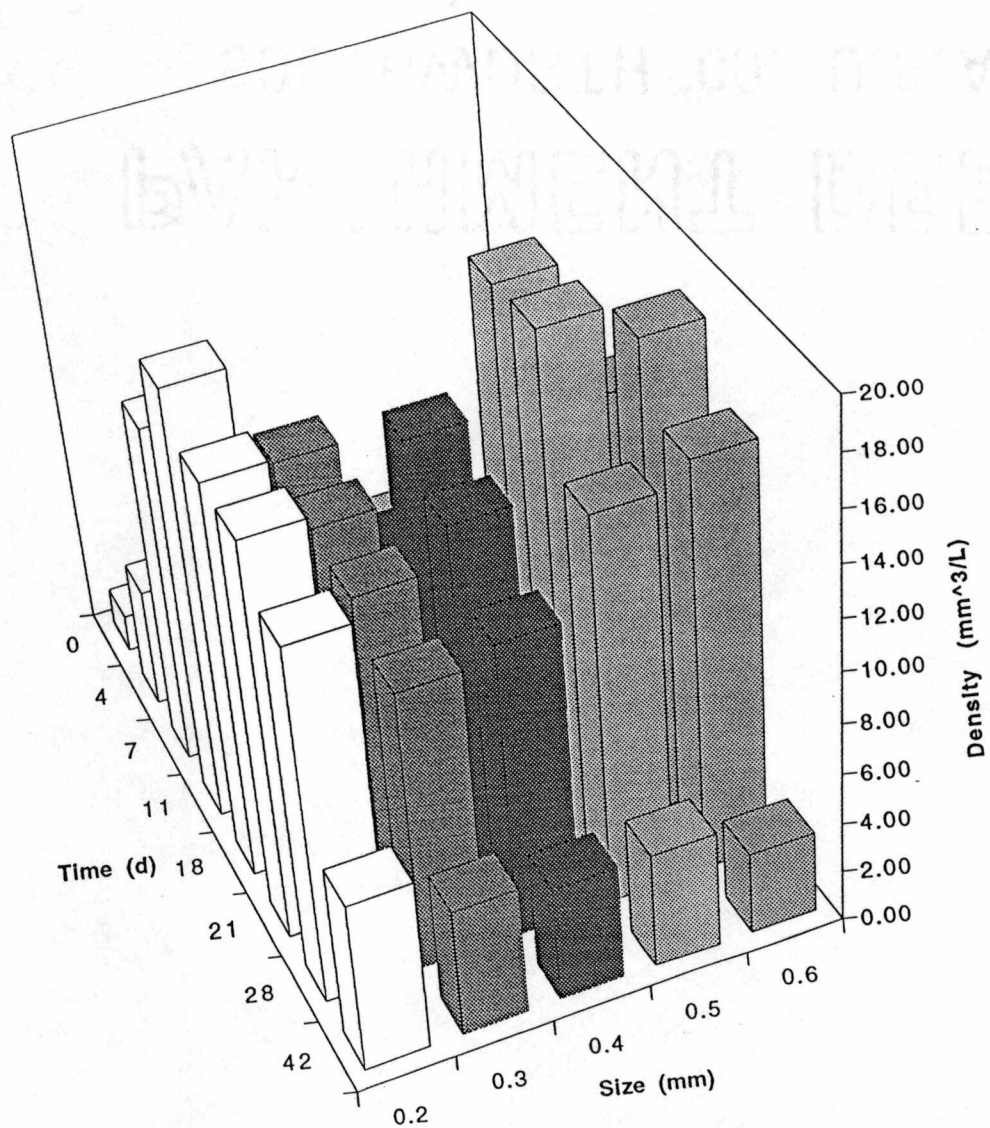
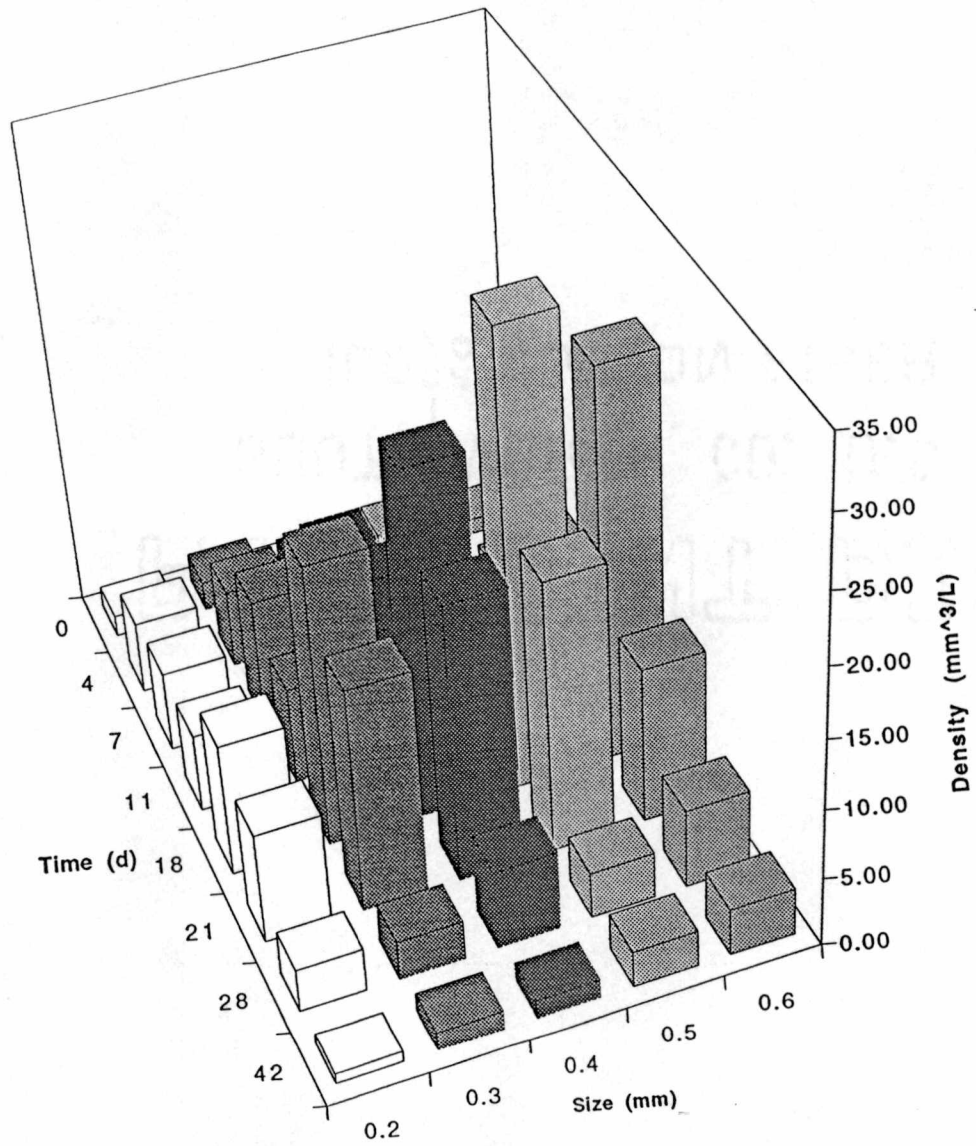


Fig.1. The functional axis represents the density of the single cell algal population using the above three forms of s . ($\circ$, s given in Eq. (2.1)), ($-$, s given in Eq. (2.3)), ($+$, s given in Eq. (2.4)).

(A)



(B)



(C)

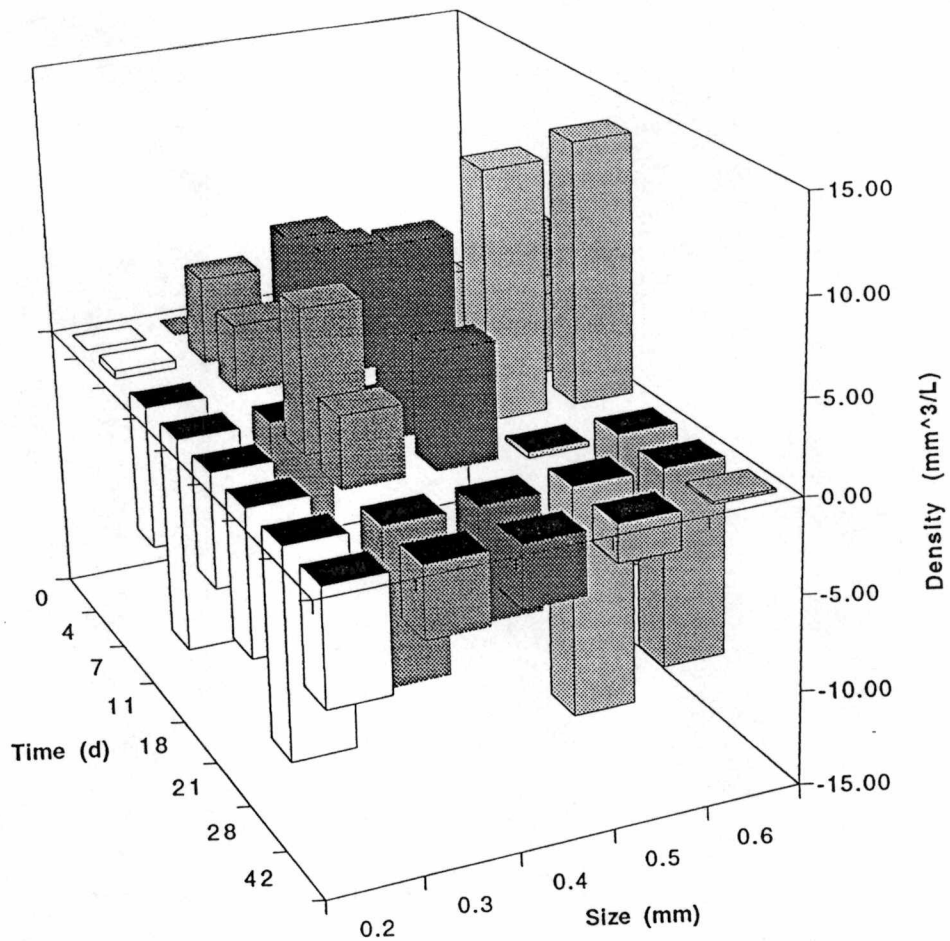


Fig.2. The functional axis represents: A) The output of the model using the stickiness function represented in Eq.(11). B) The observed data found by Riebesell (1991a). C) The difference between A) and B).

Part V

SUMMARY

In this dissertation we modeled phytoplankton dynamics by including the aggregation process. In Part II, convergence analysis for the collocation method used to approximate the solution of the aggregation integro-differential equation was presented. An inverse method for estimating the "stickiness parameter" in the aggregation equation was developed.

In Part III, an individual model that describes the life history of a single phytoplankton cell was developed. This individual model together with the aggregation process was incorporated in the phytoplankton-grazer community model. The simulation results show that the resource-consumer interactions are essential for obtaining the removal of organic matter from the surface layer in the observed time scales for experiments in the North Sea (Riebesell, 1991a,b). A change in the initial density of the grazers can lead to a change in the length of the bloom. The relationship describing the number of cells in an aggregate of certain size should be re-investigated, since our model output is sensitive to this relationship. It is also important to get information on the number of living cells in each aggregate, because an increase in this number enhances the aggregation process. The size of the phytoplankton cell is important because different cell sizes results in different aggregate distributions. Increasing the depth of the surface layer and a higher initial nutrient concentration enhanced aggregation.

In Part IV of this dissertation we used the inverse method discussed in Part II to estimate the "stickiness parameter" using the observation data found by Riebesell (1991a,b).

In our modelling effort we have included only the "essential" biological and physical processes and neglected some issues that could be important in the dynamics of the phytoplankton population when the aggregation process is included. In the next section we discuss processes that have not been included in our models and indicate future research issues.

Future research issues

- Estimation of the "stickiness parameter" using the observed data obtained by Alldredge et al. (1993). An inverse methodology similar to that used in Part IV of this dissertation will be used. This data differs from Reibesell data (1991a,b) since that nutrients are limiting in this case whereas they appear to be abundant in Riebesell's data. This estimation allows us to compare the "stickiness parameter" when nutrients are limiting to the case when nutrients are not limiting.
- Temperature and light affect the individual phytoplankton cell. In order to describe light effects, the vertical location of the cell in the ocean should be represented. This requires addition of a new dimension to our population model; hence, $\rho(t, x)$ becomes $\rho(t, x, h)$, where h is the vertical location of an

aggregate of size x at time t . The growth of each cell depends on its vertical location because the light availability is a function of depth. In discrete form one can treat this problem similar to the nonspatial one. Here the several surface layers stacked on top of each other. The matter lost from the upper layer due to sinking is an input to the layer directly below.

The following are problems that are of research interest.

- Mathematical analysis of a spatially heterogeneous model obtained from adding the vertical location dimension. It is expected that this problem can be treated similarly to that reported in Ackleh et al. (1994).
- Obtaining an estimate on the number of living cells in an aggregate using inverse methodology similar to that discussed in Ackleh et al. (1994). It has been suggested by our model results that it is important to get information on this number because it affects the aggregation process.
- Since our model results imply that resource-consumer interactions are very important to obtain observed time scales for the bloom period, an individual based model for the zooplankton seems an appropriate modification for our model. An approach similar to that used by Hallam et al. (1990) for modeling *Daphnia* might be appropriate to use.
- Investigation of the role of bacteria. It has been suggested (Riebesell, 1991a,b; Biddanda 1985) that bacteria plays a role in bonding particles together in

aggregates.

- The effect of the shape of the aggregate on the coagulation kernel and "stickiness function". In the present aggregates are assumed to be spherical. Logan and Wilkinson (1991) suggested the use of fractal dimension theory for the description of the aggregates sizes.
- Sensitivity analysis of the estimation of α to all parameters.

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APPENDICES

Appendix I: Numerical Procedure and Approximation Error

In this Appendix, we describe the flow scheme for the numerical routine employed to analyze the plankton community with aggregation. Divide the size range into N evenly spaced intervals starting with x_2 to the maximum range required and choose $x_1 = 2v_{min}$, then $\rho(t, x_k)$ represents the density of aggregates of size x_k . We start with initial distribution of single cells, i.e, $\rho(t, x_i) = 0$ for $i \neq 1$ and define v_i , $i = 1 \cdots L$, to be the volume of the cell ($v_{min} \leq v_i \leq 2v_{min}$). In our simulation, the interval $[v_{min}, 2v_{min}]$ is divided into 10 evenly spaced intervals v_i $i = 1, 2 \cdots 10$. The relationship $cell\ number = (\frac{d_{x_k}}{d_{x_1}})^{\frac{1}{0.44}}$ developed by Jackson (1990) for estimating the number of cells of diameter d_{x_1} in an aggregate of diameter d_{x_k} is used.

The LSODE package (obtained from NETLIB) is used to step forward in time for a random short period t_1 , to yield an approximation for $\rho(t, x_1) \rho(t, x_2) \cdots \rho(t, x_N)$ at time t_1 . A check to see how many cells are ready to divide according to the individual model is performed. The number of new cells is added to the single cell density $\rho(t, x_1)$ and this process is repeated until final time required is achieved. The algorithm below diagrams this process.

Define:

$cell\ number \times track_{ij} =$ The total number of cells with volume v_i in all aggregates of volume x_j

$trans_{ij}$ = The fraction of cells with volume v_i in aggregates of volume x_j (at the initial time this matrix is uniform, i.e, $trans_{ij} = \frac{1}{L}$)

$$START \rightarrow \begin{pmatrix} \rho(t, x_1) \\ \rho(t, x_2) \\ . \\ . \\ . \\ \rho(t, x_N) \end{pmatrix} \xrightarrow{O.D.E \text{ solver } LSODE} \begin{pmatrix} \rho(t, x_1) \\ \rho(t, x_2) \\ . \\ . \\ . \\ \rho(t, x_N) \end{pmatrix} \xrightarrow{\rho(t, x_j) \times trans_{i,j}}$$

$$\begin{pmatrix} track_{11} & track_{12} & & track_{1N} \\ track_{21} & track_{22} & & track_{2N} \\ . & . & . & . \\ . & . & . & . \\ . & . & . & . \\ track_{L1} & track_{L2} & & track_{LN} \end{pmatrix} \begin{array}{l} \text{If } v_i = 2v_{min} \text{ then} \\ track_{i1} = track_{i1} \\ + \sum_{j=1}^N \text{cell number} \times track_{ij} \end{array}$$

$$\begin{pmatrix} track_{11} & track_{12} & & track_{1N} \\ track_{21} & track_{22} & & track_{2N} \\ . & . & . & . \\ . & . & . & . \\ . & . & . & . \\ track_{L1} & track_{L2} & & track_{LN} \end{pmatrix} trans_{ij} = \frac{track_{ij}}{\sum_{i=1}^L track_{ij}}$$

$$\begin{pmatrix} trans_{11} & trans_{12} & & trans_{1N} \\ trans_{21} & trans_{22} & & trans_{2N} \\ . & . & . & . \\ . & . & . & . \\ . & . & . & . \\ trans_{L1} & trans_{L2} & & trans_{LN} \end{pmatrix} \rho(t, x_j) = \sum_{i=1}^L track_{ij}$$

$$\begin{pmatrix} \rho(t, x_1) \\ \rho(t, x_2) \\ . \\ . \\ . \\ \rho(t, x_N) \end{pmatrix} \xrightarrow{\text{go to } START}$$

Notice that if the initial distribution is uniform in the sense that the number of cells having different volumes is the same at the initial time, then because cells in larger aggregates are composed from cells in smaller aggregates, they inherit the proportionality of the cell number type. Hence, we keep track of the column $trans_{i1}$ in the $trans$ matrix.

The choice of the collocation method over other methods is primarily because of the simplicity of implementation. The accuracy and the order of convergence obtained from using the collocation method depends on both, the interpolation accuracy and the accuracy of the numerical method used to approximate the resulting differential equation system. For example, if the solution $\rho(t, x) \in C^4[0, A]$ and cubic splines are used for interpolation and a 4th order Runge-Kutta is used for solving the differential equation system, then it is easily deduced from the proof of Theorem 2.1 that the order of convergence of the collocation method in $\|\cdot\|_0$ is 4th order. A comparison between this method and the sectionalization approach used by Jackson and Lochmann (1992), is presented in Gelbard et al. (1980). A numerical simplification is achieved using a uniform mesh for the following reason. Since $x_j - x_k = x_{j-k}$ if the mesh is uniform then no interpolation is needed at

every time step, since we need only information at the grid and not in between. This even makes the collocation simpler, faster and more attractive to use. The disadvantage of the uniform mesh is that if the single cell radius is small then, this increases the number of differential equations that must be solved. But this disadvantage can be avoided by choosing a uniform mesh except for the first grid point. Then, only one interpolation operation is required for every time step since $x_j - x_k = x_{j-k}$ for $k \neq 1$.

To test our numerical scheme we used following aggregation equation:

$$\frac{\partial \rho(t, x)}{\partial t} = \frac{1}{2} \int_0^x \beta(x-y, y) \rho(t, x-y) \rho(t, y) dy - \rho(t, x) \int_0^\infty \beta(x, y) \rho(t, y) dy \quad (1)$$

with initial condition:

$$\rho(0, x) = \frac{N_0}{x_0} e^{-x/x_0}$$

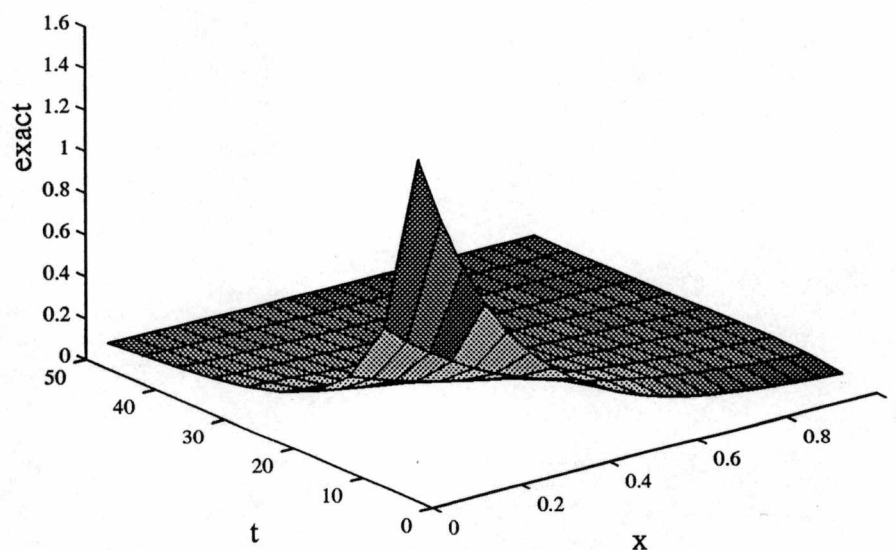
where N_0 is the total initial number of particles, x_0 is the mean initial volume. If $\beta(x, y) = \beta_0$ a constant then the exact solution is given in Gelbard et al. (1980) to be:

$$\rho(t, x) = \frac{4N_0}{x_0(N_0\beta_0t + 2)^2} \exp\left(-\frac{2x}{x_0(N_0\beta_0t + 2)}\right)$$

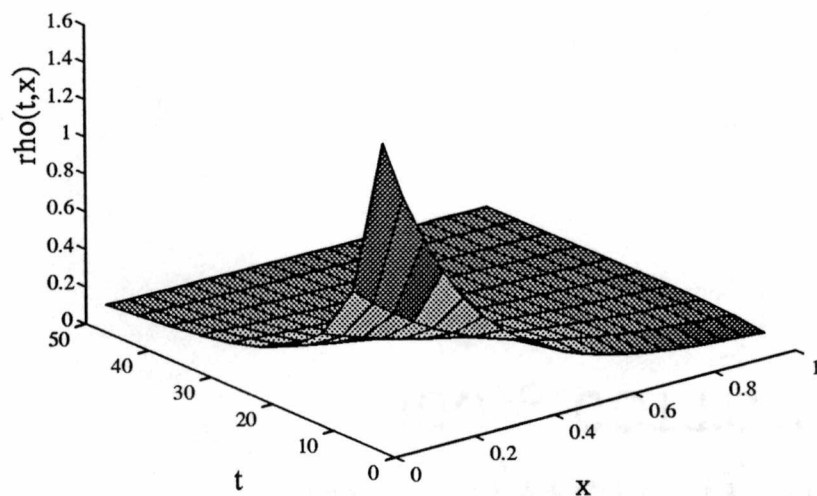
In Fig. 1 and 2 we chose $x_0 = 0.1$ and $N_0 = 1$. Fig.1 represents the approximation of this equation using the collocation method versus the exact solution. Since one can only integrate on a finite time numerically, Fig. 2 represents the

difference in error when we integrated over a larger interval than in Fig. 1 and all other conditions are the same. It seems that the error that arises from a finite interval is really important so one should make sure that the interval integrated over causes only a small error in the approximation.

(A)



(B)



(C)

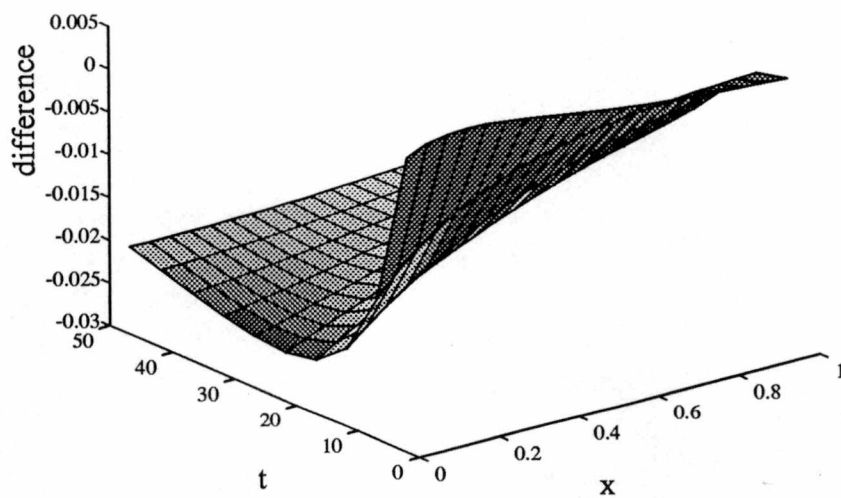
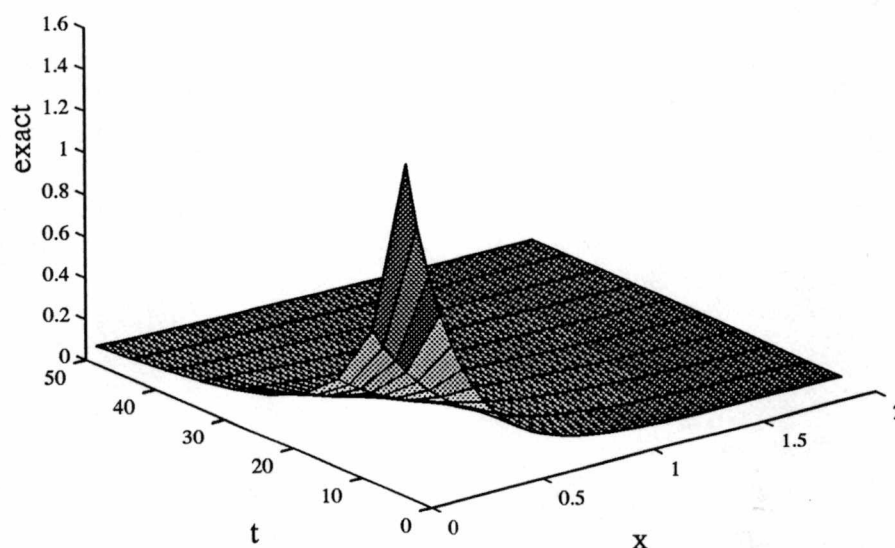


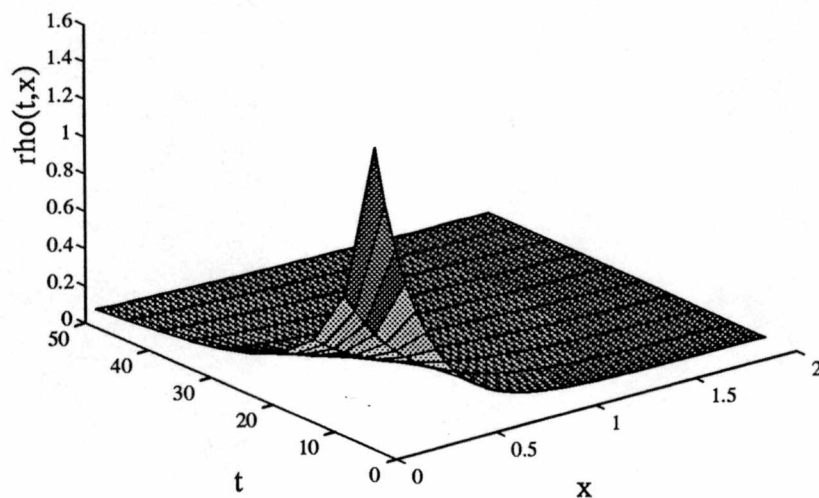
Fig. 1. The functional axis represents: A) The exact solution of (1). B) The approximation solution of (1) using the collocation method. C) The difference between the exact and the approximation solutions of (1).

In Fig. 3 we chose $x_0 = 0.05$ and $N_0 = 1$. A lower value for x_0 reduces the finite time integration error to a negligible one so this explains the error that occurs from approximation only. We ran several simulations, in these simulations we chose the size step half of the former one and showed that the error reduces as one reduces the mesh size. The standard 2-norm was used to calculate the error.

(A)



(B)



(C)

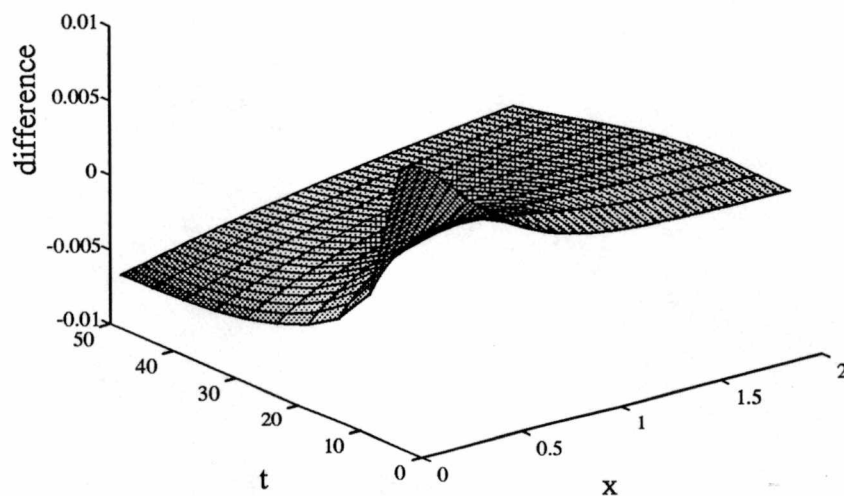


Fig. 2. The effect of finite interval length on the approximation. The functional axis represents
A) The exact solution of (1) B) The approximation solution of (1) using the collocation method
c) The difference between the exact and the approximation solutions of (1).

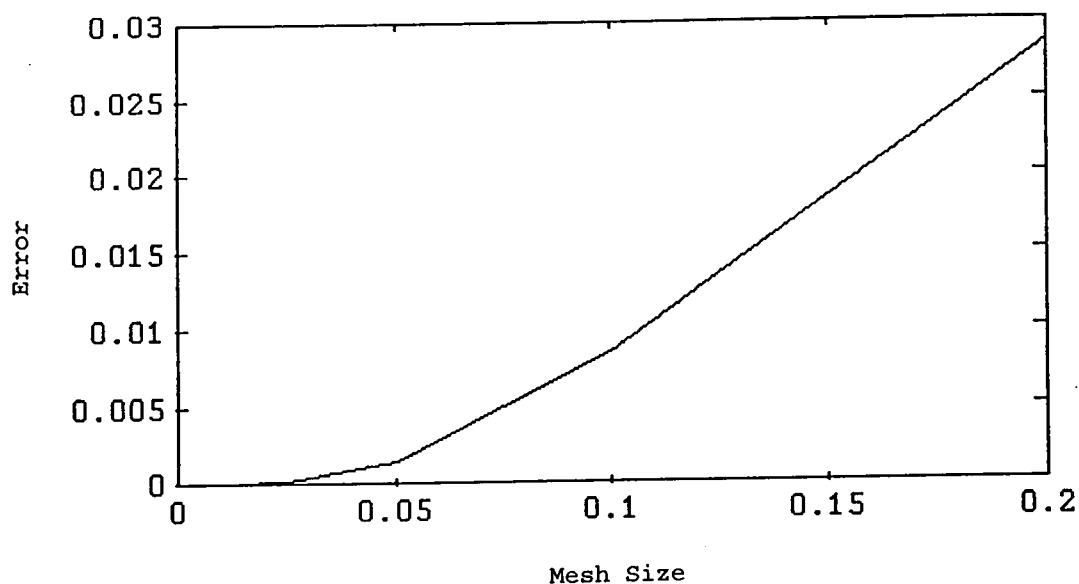


Fig. 3. The functional axis represents the approximation error.

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2. Jackson G. and S. Lochmann (1992) *Effect of coagulation on nutrient and light limitation of an algal bloom*, *Limnology and Oceanography*, **37** 77-89.
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Appendix II: Effects of initial zooplankton density on the bloom length

In this Appendix the dynamics of both zooplankton and phytoplankton population are represented using two different initial zooplankton densities ($0.5 \text{ \#}/L$, $0.05 \text{ \#}/L$). The carrying capacity model from Part III of this dissertation is used in the following simulations. Similar results hold for the zooplankton linear model. In Fig. 1 the dynamics of the phytoplankton single cells is presented using both initial densities. Fig. 2 represents the dynamics of zooplankton using the above two initial densities. Fig. 3 and 4 represents the dynamics of aggregates using the above initial densities for zooplankton. The results show that higher initial density for zooplankton results in shorter bloom length for phytoplankton.

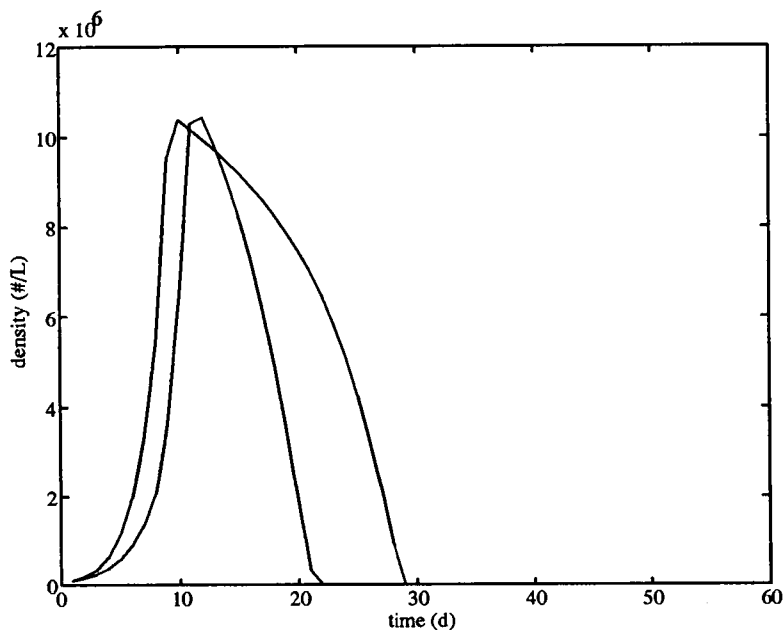


Fig. 1. The functional axis represents the density of single cells using different values of zooplankton initial density ($0.5 \text{ \#}/L$, $0.05 \text{ \#}/L$).

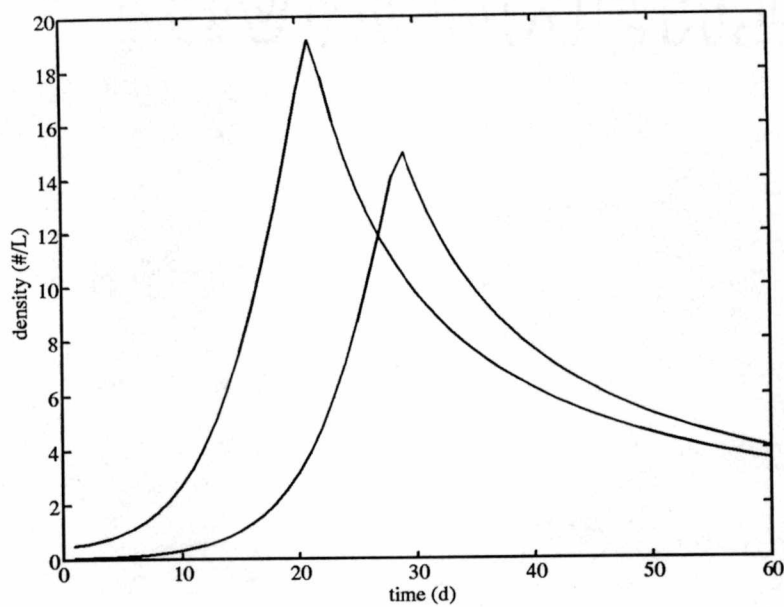


Fig. 2. The functional axis represents the density of zooplankton using different values of zooplankton initial density (0.5 #/L, 0.05 #/L).

(C)

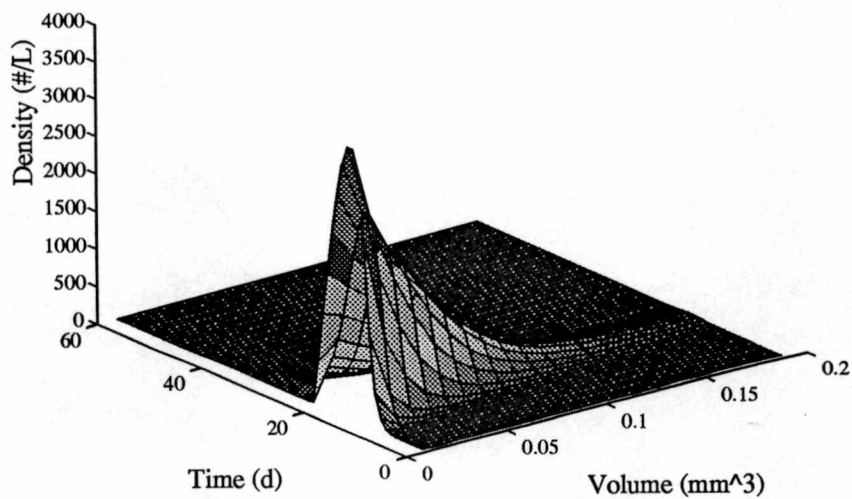


Fig. 3. The functional axis represents the density of aggregates using the value 0.5 #/L for zooplankton initial density.

(C)

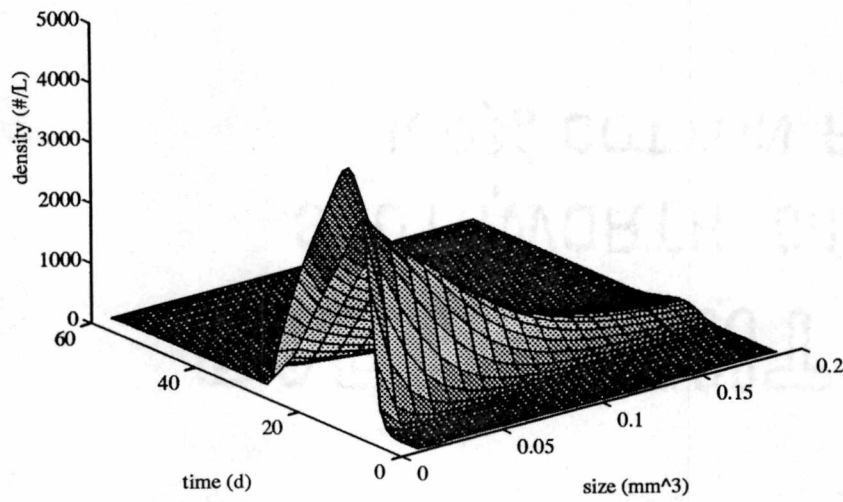


Fig. 4. The functional axis represents the density of aggregates using the value 0.05 #/L for zooplankton initial density.

VITA

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