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I am submitting herewith a thesis written by Nicole Billie Puckett entitled "The Role of Fractal Dimension in an Algal Aggregation Model." I have examined the final copy of this thesis for form and content and recommend that it be accepted in partial fulfillment of the requirements for the degree of Master of Science, with a major in Mathematics.

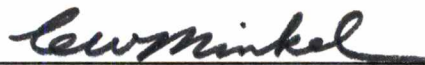


Thomas Hallam, Major Professor

We have read this thesis
and recommend its acceptance:



Accepted for the Council:



Associate Vice Chancellor and
Dean of The Graduate School

The Role of Fractal Dimension in an Algal Aggregation Model.

A Thesis
Presented for the
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Abstract

Aggregation plays an important role in the transfer process of matter from the surface of the ocean to the ocean floor and thus may contribute to a significant sink of carbon. Mathematical models have been developed to help scientists understand more about the aggregation process. This study modified a model to better represent the shape of the aggregate using fractal dimension and to include reproduction of live cells that are inside an aggregate. A least squares methodology was used to estimate the fractal dimension and yielded a value of 2.8. This value indicates that the aggregates are close to three dimensional but are not solid spheres.

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Chapter 1

Introduction

Aggregation, the formation of larger particles due to the combining of smaller ones, plays a key role in the transfer of matter from the surface of the ocean to the ocean floor because the heavier the particle, the more likely it is to sink. This transfer process is of interest due to its relationship to the carbon cycle. Any carbon on the ocean floor is permanently lost from the system unless it is recycled in some way. Thus, aggregation may be a potentially significant sink of carbon.

In 1993, an experiment was performed in Santa Barbara to help scientists understand more about the aggregation process. In this experiment a 1400 liter, cylindrical tank was filled with 1150 liters of sea water. Over fourteen days the tank was monitored for aggregates of different sizes. Sixteen sets of data were taken during the fourteen day period. Data was taken every other day for the first eight days and then every twelve hours thereafter. From this experiment, aggregation of phytoplankton cells could be observed over time. For more information on the SIGMA tank experiment see Alldredge et. al., 1995.

The purpose of this thesis was to consider and mathematically model the morphology of aggregates as well as to correct a current model of the reproduction of cells inside an aggregate.

1.1 The Biology

In their 1994 paper, Ackleh et al. presented an aggregation model. This model tracks the growth and reproduction of the individual phytoplankton cells as well as calculates the number of aggregates in specific size classes for a given time. Thus, their model can be separated into two main parts: one part for individual cells and one part for aggregates.

When preparing an individual cell model it is helpful to choose a specific cell as a reference cell in order to make the model more realistic. Because diatom cells are fairly universal, were the dominant species in the SIGMA tank and play an important role in aggregation, they were chosen as the reference cell for this model. Diatoms have two characteristics that will play an important role in the model. First, the diatom cell grows inside a siliceous frustule or test. This test remains invariant in size while the cell inside grows over time. Second, because of their unique morphology, when diatoms reproduce or collide and stick, they tend to form linear chains.

The growth and reproduction of the phytoplankton cells is dependent on the availability of nutrients such as nitrogen, phosphorous, and silica. The limiting nutrient, in the Santa Barbara experiment, is nitrate. The tank and model are initialized by a single pulse of nitrate. This means the nutrient concentration, which is depleted by the cells, is never increased by an outside source except for the initial amount. A graph of nutrient concentration versus time for the tank experiment is

presented in Figure 1. A diatom cell is assumed to reproduce after its carbon content doubles. When this happens, the cell asexually divides leaving two cells of the same size with the same carbon content. Thus, the model must track, not only the level of nutrients, but also the carbon content in each cell.

The second part of the model tracks the number of aggregates in specific size classes, the first of which includes the single cells or "free cells". As noted above, the number of single cells increases with reproduction. It also increases when larger aggregates collide and break up. On the other hand, the number of free cells will decrease when they collide with another aggregate and stick, thus becoming part of the aggregate. Also, some cells will sink and after dropping below a specified level, they will die due to lack of sunlight, thus decreasing the number of cells.

In a similar manner, the number of multicellular aggregates of a particular size may increase or decrease due to aggregation or sedimentation. Larger aggregates are more prone to sedimentation because they are heavier.

A multicellular aggregate may also grow when a cell that is part of an aggregate reproduces. The model presented in Ackleh et. al. assumed that when a cell reproduced inside an aggregate one cell stayed in the aggregate and one cell became a free cell. In Prowe's 1995 thesis, the model was modified to the assumption that when reproduction in the aggregate occurs, at least one of the daughter cells remains in the aggregate while the other cell has probability $1-q$ of becoming a free cell, and a probability q of remaining in the aggregate. Reproduction in aggregates is explained in greater detail in the next chapter.

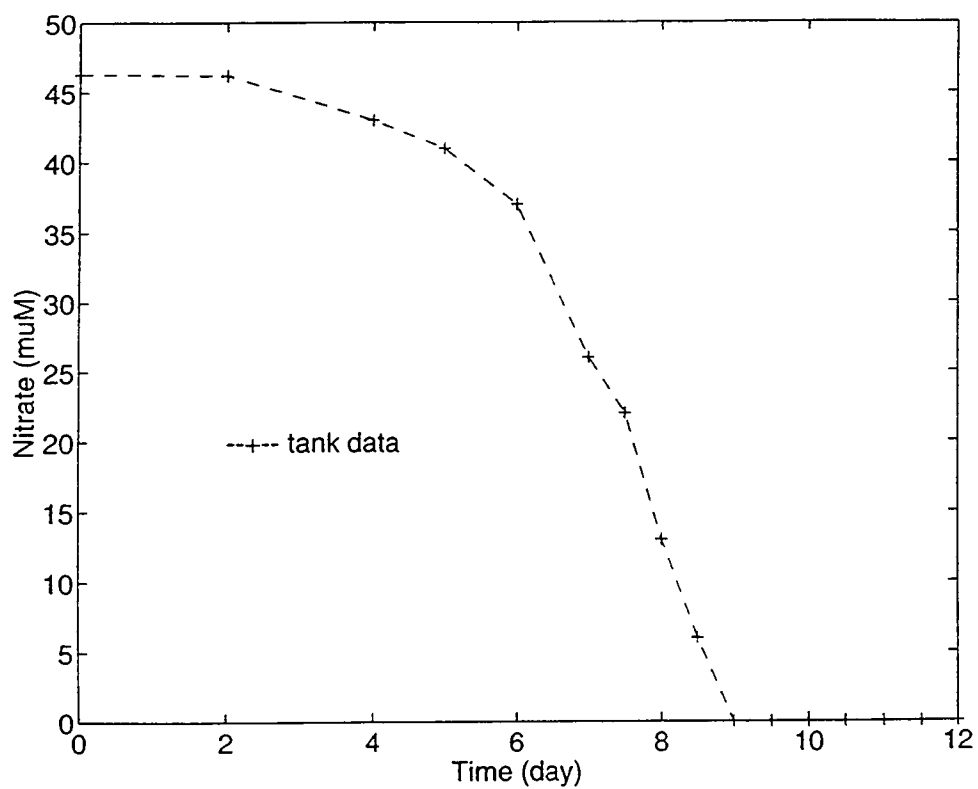


Figure 1
Depletion of Nutrients in the SIGMA tank experiment

There is an external factor, consumption, included in this model that influences the number of aggregates in a particular size class. The consumers, zooplankton, ingest aggregates in a particular size range with the larger aggregates being less apt to be consumed.

A diagram which shows all the components in this model and how they relate is presented in Figure 2.

1.2 The Foundation of the Model

1.2.1 Individual Model

If $C(t)$ is the content of carbon at time t in a diatom cell, then the rate of change of carbon with respect to time is the assimilation rate minus the maintenance rate. Since diatoms grow inside a siliceous frustule with a fixed volume, v , and a constant surface area, $v^{2/3}$, the assimilation rate of carbon is assumed to be proportional to $v^{2/3}$ with proportionality constant a . The maintenance rate of a cell is considered proportional to the carbon content with a constant of proportionality b . Both the assimilation rate and maintenance rate are dependent on the availability of nutrients in a manner so that the ultimate cell size is independent of nutrient availability. Thus the rate of change of carbon with respect to time is assumed by

$$\frac{dC}{dt} = \frac{N}{k_N + N} (av^{2/3} - bC)$$

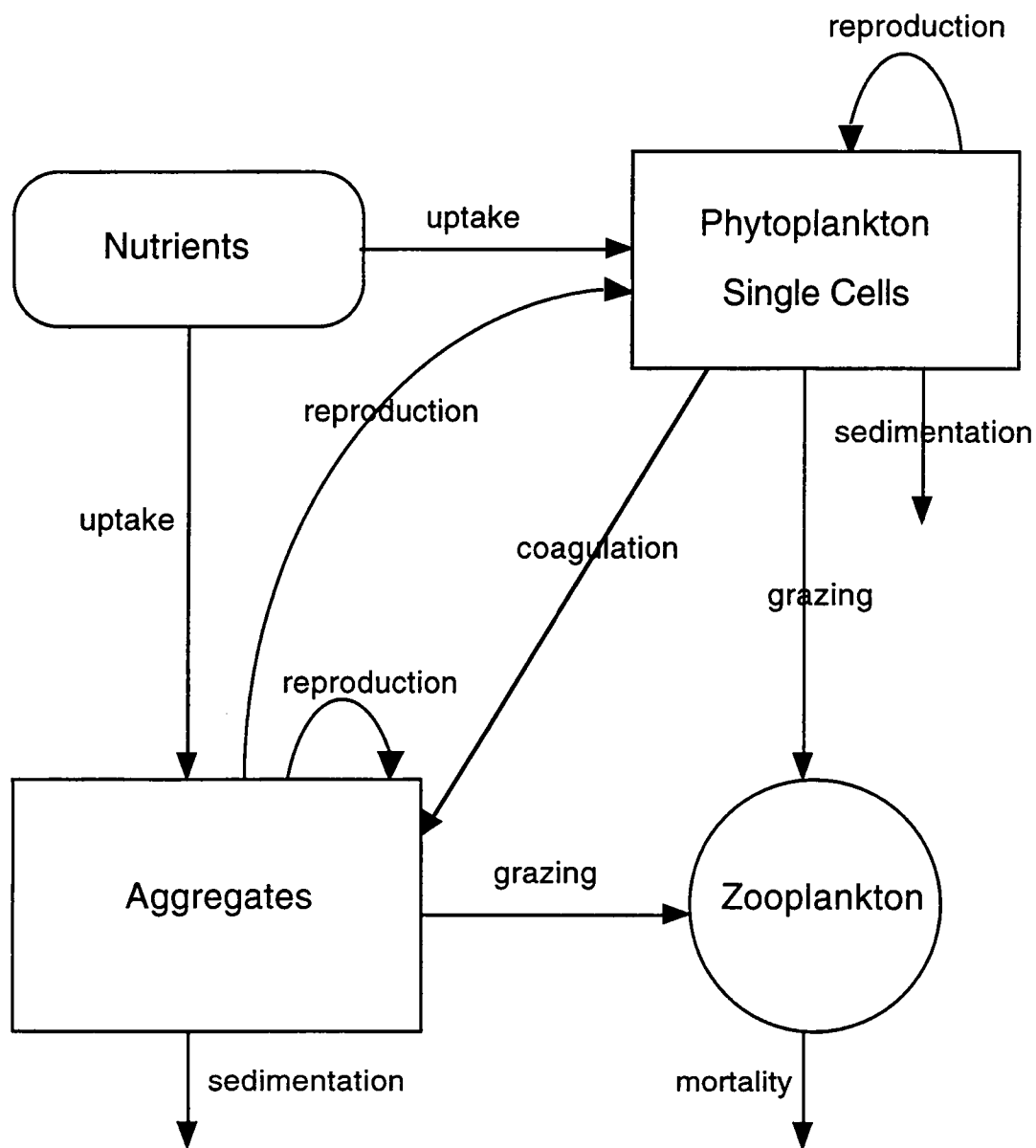


Figure 2
Aggregation Diagram

with the initial condition

$$C(0) = C_{\min},$$

where N is the amount of the limiting nutrient (nitrate) and k_N is a half saturation constant of that nutrient. When the amount of carbon in a cell doubles, i.e. when $C=2C_{\min}$, the cell reproduces asexually into two cells each with half the amount of carbon that the original cell had.

Values for a, b, v, k_N , have been found in previous research. A list of their values, units and references are given in Table 1 along with other parameters used in this model.

1.2.2 Aggregation model

The aggregation model is composed of four different terms. The first two describe the change in aggregate size due to collisions. If $\rho(t, x)$ is the density of aggregates at time t with volume x ($\#mm^3l^{-1}$) then the rate of change of $\rho(t, x)$ with respect to time is

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

where $\alpha(x, y)$ is the probability of an aggregate of size x sticking to an aggregate of size y after colliding (no dimension), $\beta(x, y)$ is the rate of collision times the contact

Table 1 Parameter Values and Units			
Symbol	Interpretation	Value (unit)	Source
v	volume of cell	$4000(\mu m^3)$	
x	volume of aggregate	(mm^3)	
t	time	(d)	
N	nitrate concentration	(μM)	
N ₀	initial nitrate concentration	$45.0(\mu M)$	
k_N	half saturation constant	$0.5(\mu M)$	Scheffer 1991 Jackson and Lochmann 1992
a	cell growth rate	$(\mu m \mu mm^{-2/3} d^{-1})$	derived in Ackleh, Hallam, and Smith 1994
b	cell maintenance	$0.0084(d^{-1})$	Lancelot, Billen, and Barth 1991
C _{min}	initial carbon mass of cell	$208.4(pg)$	
$\rho(t, x)$	density of aggregates	$(\#mm^{-3}l^{-1})$	
$\beta(x, y)$	coagulation kernel	$(cm^3t^{-1}\#^{-1})$	
q	portion of new cells sticking to aggregate	varied	
p	portion of live cells in aggregate	varied	

efficiency for two particles ($cm^3 t^{-1} \#^{-1}$) and A is the maximum aggregate volume size considered in the model. Notice the first term of the above equation describes the rate at which aggregates between size x and $x+dx$ are formed due to collision and the second term describes the rate at which, due to collision, aggregates between size x and $x+dx$ are lost.

There are two main kinds of motion that cause aggregates to collide, differential settling and shear motion. Thus $\beta(x, y)$ is made up of two terms,

$$\beta(x, y) = \beta^d + \beta^s,$$

where

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

and

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

β^d is the rate of collision due to differential settling and β^s is the rate of collision due to shear motion. In the above equations d_x is the diameter of an aggregate of size x , ω_x is the settling velocity of an aggregate of size x , ε is the energy dissipation rate, and ν is the kinematic viscosity. $EC_{x,y}^d$ and $EC_{x,y}^s$ are the contact efficiencies for differential settling and shear motion respectively given by

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

and

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

where

$$EC_0 = \frac{1}{\exp(-0.1)} ,$$

$$d_{\min} = \min(d_x, d_y) \text{ and } d_{\max} = \max(d_x, d_y).$$

The third term in the aggregation model depicts a loss of aggregates due to sinking. As aggregates grow, due to collisions, they become more dense and hence sink. Once they sink to a certain level, D , the aggregates can no longer receive light and die. If $\omega(x)$ is the sinking velocity of an aggregate of size x and R is the radius of the aggregate then the loss of aggregates due to sinking can be described by

$$\rho(t, x) \frac{\omega(x)}{D}$$

where

$$\omega(x) = f_\rho \xi R^{1.17} .$$

ξ here represents a curve fit parameter and f_ρ represents a fall scale parameter.

In the ocean, aggregates are a food source for zooplankton and so the fourth term of the model is a loss of aggregates due to the grazing of zooplankton. In order to express this loss it is helpful to understand a simple model of zooplankton. If zooplankton can ingest aggregates at a rate of p_z with an assimilation efficiency of δ then the rate of change of the density, z , of zooplankton with respect to time is

$$\frac{dz}{dt} = p_z \delta \frac{\int_0^A f(x) \rho(t, x) dx}{\int_0^A f(x) \rho(t, x) dx + k_p} z - m z^r$$

where $f(x)$ is the probability of an individual zooplankton ingesting an aggregate of size x and m is the mortality rate. r is either 1 or 2, 1 for a first order grazing and 2 for logistic grazing. k_p is a trophic response half saturation constant. It is important to note that only small aggregates can be ingested and hence for $x > x_{\max}$, $f(x) = 0$. After looking at the zooplankton model, the loss of aggregates due to grazing is

$$p_z \frac{f(x) \rho(t, x)}{\int_0^A f(x) \rho(t, x) dx + k_p} z.$$

The aggregation model with all four terms is

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

$$-P_z \frac{f(x)\rho(t,x)}{\int_0^A f(x)\rho(t,x)dx + k_p} z.$$

1.3 Objectives

One objective of this study was to correct the reproduction routine in a Fortran code so it would accurately track the growth of an aggregate due to cell division. Although the concept was correct in the previous code, the method employed was inadequate.

A second objective of this study was to adjust the aggregation model to better represent the morphology of aggregates. Previously, for simplicity, the model made the assumption that aggregates were exactly spherical in shape but, as mentioned earlier, the diatom cells generally form more of a linear chain rather than a sphere. From a different perspective, one might say that the diatom chains are porous compared to the perfect sphere, i.e., if you placed the diatom chain inside the smallest sphere possible, then there would exist pockets of water inside the sphere where there are no diatom cells. The porosity of an aggregate affects its coagulation rates in several ways (Jackson, 1995; Jiang and Logan, 1991). Firstly, more porous particles have slower settling velocities than particles that are less porous. The slower settling velocities may decrease the chance of colliding by differential sedimentation. Secondly, more fluid will flow through an aggregate with higher porosity. This increases the chance of particle contact with the aggregate by shear motion. Thus,

modeling the porosity of an aggregate should improve the coagulation rates by making them more realistic.

1.4 Fractal Dimension

One tool which is used to help describe the porosity of an aggregate is the fractal dimension. In order to understand what the fractal dimension is or how it is found, it helps to consider a few basic illustrations.

The first illustration considers a line one unit in length. The first step in “measuring” this line is to define a closed ruler. In this case a linear ruler, ε units in length, works nicely. The second step is to note how many of these rulers it takes to cover the line. Here it takes $1/\varepsilon$ rulers to cover a line one unit in length. It is good to note at this point that ε is raised to the first power.

The second illustration regards a one by one unit square. So we define our ruler to be a square with a side of length ε . In this case, the unit square could be covered with $(1/\varepsilon)^2$ or $1/(\varepsilon)^2$ rulers. Now in this second illustration ε is raised to the second power.

From these two illustrations, one might guess that the exponent of the general length ε is of some importance and, in fact, it is.

If $N(\varepsilon)$ is the number of closed rulers it takes to cover a subset S of R^n where $n=1,2,3$ and if

$$N(\varepsilon) = C \left(\frac{1}{\varepsilon} \right)^D,$$

then solving for D it is seen that

$$D = \frac{\ln N(\varepsilon)}{\ln(1/\varepsilon)} - \frac{\ln C}{\ln(1/\varepsilon)} \approx \frac{\ln N(\varepsilon)}{\ln(1/\varepsilon)}$$

when ε is very small. Thus we define the capacity dimension of S to be

$$\dim_c S = \lim_{\varepsilon \rightarrow 0} \frac{\ln N(\varepsilon)}{\ln(1/\varepsilon)}$$

if the limit exists. If a subset S has a capacity dimension and it is not an integer then S has a fractal dimension. A good example of a subset with fractal dimension is the von Koch curve. For more details see (Lauwerier 1991).

It can be seen that the fractal dimension is related to the porosity of an aggregate. The smaller the fractal dimension the more porous the aggregate is. For example, if an aggregate has a fractal dimension between 1 and 2 but closer to 1 than 2, then the aggregate is closer to being linear than being a plane. Hence it is more porous than an aggregate of higher dimension.

Chapter 2

Methodology

2.1 Reproduction in the Model

This aggregation model starts with an initial number of free cells and with no aggregates. The carbon content of these free cells varies from the minimum amount, $C_{\min}$, to twice the minimum, $2C_{\min}$, which is when the cell will reproduce. In particular, the initial cells are divided into n different types where each type has a different carbon content. Hence, a cell of type i has an initial carbon content of $C_{\min} + \frac{i-1}{n-1} C_{\min}$. Thus, all cells will not reproduce at the same time but only those cells of the same type will simultaneously reproduce. Hence, the subroutine for reproduction is called every hour to check the carbon content of each type of cell.

During the hour between reproduction times, aggregation is taking place. It is assumed that the proportion of cells of type i in an aggregate of size j is the same after the hour of aggregation as it was before the hour. If a size class was empty before aggregation but not after, then it is assumed that these aggregates will have an equal amount of each type of cell. The proportion of cells will change only after reproduction has occurred.

The first step of the reproduction routine is to check the carbon content of the single cells. Those that have twice the minimum amount of carbon divide into two identical free cells.

The second step is to check the carbon level in living cells inside an aggregate. It is assumed that only a percent, p , of the cells in an aggregate are alive while the rest of the cells are dead. Thus, if there are x number of cells that make up the aggregate only px are alive and have the potential of reproducing. When a cell in an aggregate reproduces, one of the daughter cells remains attached to the aggregate while the other cell has probability q of sticking and probability $1-q$ of becoming a free cell. Thus, if the cells of type i are ready to reproduce, then the number of free cells will increase by $px(1-q)$ (proportion of cells of type i in an aggregate of size j). In the same manner the size of the aggregate will increase by pxq (proportion of cells of type i in an aggregate of size j).

Once the aggregates have grown due to reproduction they must be placed in the appropriate size class. This is done by finding the values k and $k+1$ such that they are grid points and they bound the new size of the aggregates. The aggregates are then split into the two size classes k and $k+1$ by using the proportion of the distance between the new size and k and the distance between k and $k+1$. At the same time, the previous size class the aggregates occupied is cleared until filled either by reproduction or aggregation.

A sensitivity study was done on the new parameters p and q to see the effect a slight change in the parameters would have on the model output. Details of the sensitivity study are found in section 1 of Chapter 3.

2.2 Fractal Dimension in the Model

In Jackson's 1995 paper, he presented an "outer radius" which involves the fractal dimension, D , of the aggregate. This outer radius could be used in place of the Euclidean radius, which is the radius an aggregate would have if it were a perfect sphere with porosity zero. The outer radius, $\hat{r}$ is defined by

$$\hat{r} = \left(\frac{D+2}{D} \right)^{\frac{1}{2}} r_g \quad (1)$$

where the radius of gyration, r_g , is the radius such that if all the mass of the aggregate was placed at the radius r_g , then the moment of inertia would remain the same.

This outer radius seems consistent with what one would expect in that if the radius of gyration stays constant, then as the fractal dimension rises the radius decreases and vice versa. If the fractal dimension decreases, then the radius increases. On the other hand, if the fractal dimension for two different aggregates is the same but the first aggregate has a larger radius of gyration than the second, then the first will also have a larger outer radius. As a first step to including fractal dimension in the aggregation model this radius was used after the following substitutions.

The radius of gyration and the Euclidean radius, r_e , are related in the following way (Wu and Friedlander, 1993)

$$\left(\frac{r_e}{r_0}\right)^3 = A\left(\frac{r_g}{r_0}\right)^D, \quad (2)$$

where r_0 is the radius of the primary particle that makes up the aggregate and A is a proportionality constant that depends on how the aggregates were formed and on the fractal dimension.

Solving equation (2) for r_g we get

$$r_g = \left(\frac{r_0^{D-3} r_e^3}{A}\right)^{1/D}. \quad (3)$$

Substituting (3) into (1) yields

$$\hat{r} = \left(\frac{D+2}{D}\right)^{1/2} \left(\frac{r_0^{D-3} r_e^3}{A}\right)^{1/D}.$$

The outer radius is now in terms of known values except for the fractal dimension and the proportionality constant A . In the model, $2\hat{r}$ replaces the diameter, d , of an aggregate. Thus, the function β is now given by,

$$\beta(x, y) = \frac{\pi(2\hat{r}_x + 2\hat{r}_y)^2}{4} |\omega_x - \omega_y| EC_{x,y}^d + 0.163 \left(\frac{\varepsilon}{v}\right)^{1/2} (2\hat{r}_x + 2\hat{r}_y)^3 EC_{x,y}^s,$$

where

$$EC_{x,y}^d = \frac{\left(\frac{\hat{r}_{\min}}{\hat{r}_{\max}}\right)^2}{2\left(1 + \frac{\hat{r}_{\min}}{\hat{r}_{\max}}\right)^2}$$

and

$$EC_{x,y}^s = EC_0 \exp \left(\frac{-0.1}{\hat{r}_{\min} / \hat{r}_{\max}} \right).$$

The terms for loss due to sinking and grazing were not altered by fractal dimension because they were eliminated for the reasons given below.

2.3 Numerical Procedures

An estimate for the fractal dimension, D , the proportionality constant, A , and the sticking coefficient, α , was found by using the inverse method of least squares to fit the output of the model to data found in the SIGMA tank experiment.

In order to compare the data from the tank experiment to the output of the aggregation model the model had to be altered in two ways. The first change was so the model would best represent the environment of the experiment and the second change was so the tank data and model output would agreed in bin size.

In the tank experiment there were no zooplankton present and therefore grazing was not a factor in the loss of aggregates. Hence, the grazing term was eliminated from the model. Similarly, there was very little loss due to sinking during the study and thus the term for sinking was also removed. Consequently, the aggregation model was reduced to the following:

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

$$-\rho(t, x) \int_0^A \alpha(x, y) \beta(x, y) \rho(t, y) dy.$$

In order to compare the output of the model to the data from the experiment, size classes of each have to correspond. The tank data was originally recorded in non-uniform bins such that each bin was twice the length of the previous one. The data was received from Ackleh in an interpolated form so that every bin size was identical. Each bin is 0.01 mm^3 in length starting with size 0.01 mm^3 and ending with size 1 mm^3 . Figure 3 presents the data from the tank experiment from day 2 to day 14 (the graph is labeled from day 0 to day 12). The aggregation model uses a non-uniform grid for its size classes and thus, in order to make a comparison, a linear interpolation was done on the model output to create uniform size classes of length 0.01.

A least squares methodology is utilized to minimize the sum of the squared differences between the data and the model output. Because of the large difference in magnitude between the densities in the smaller size classes and the densities in the larger size classes, the actual comparison was done between the log of each value. This reduces the problem of the estimation being biased towards the larger values. Thus, the inverse method used here minimized the following number

$$\sum_{i=1}^N \sum_{j=1}^M \left[\log(\phi(t_i, x_j) + 1) - \log(z_{i,j} + 1) \right]^2$$

where $\phi(t_i, x_j)$ is the output of the model and $z_{i,j}$ is the data from the tank experiment. The minimization routine LMDIF was obtained from the NETLIB library and used for this study (Garbow et. al., 1980).

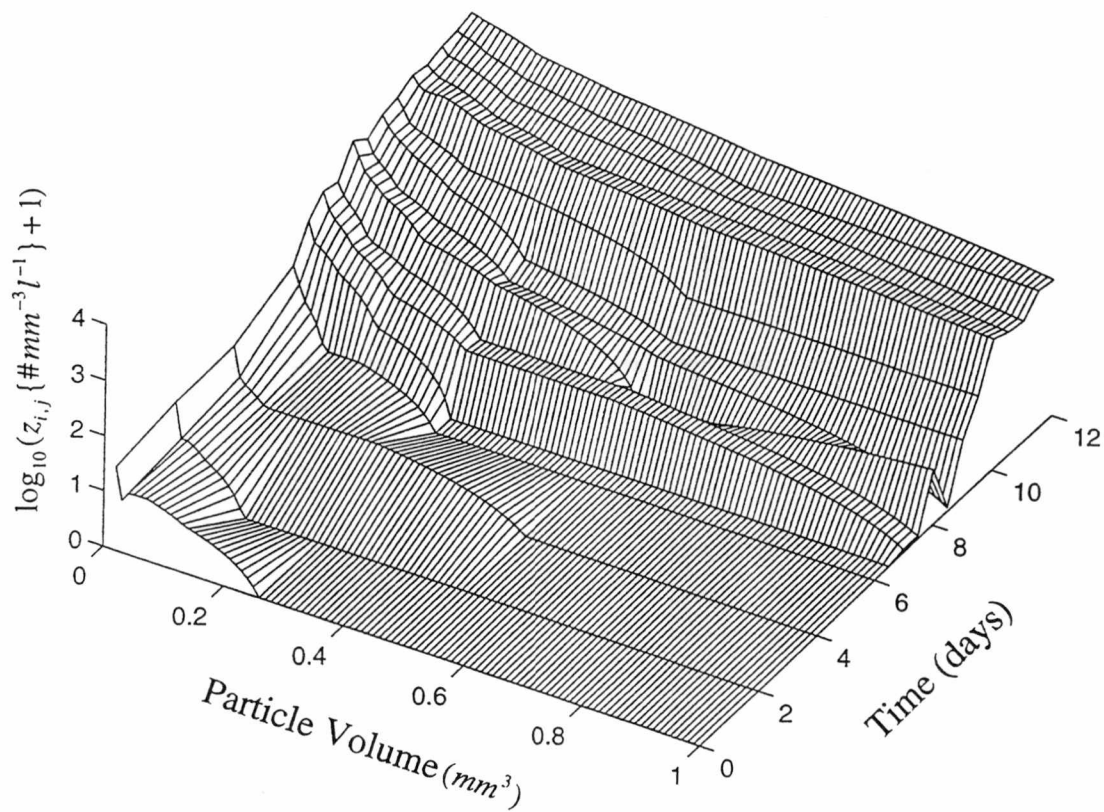


Figure 3
Graph of data from the SIGMA tank experiment

Chapter 3

Results

3.1 Sensitivity Studies

A sensitivity study was done on the new parameters, p , q , D , and A , along with the sticking probability, α , and the initial number of free cells which is denoted by fc . In the tank experiment the initial amount of nutrients was approximately $45.0 \mu M$ which is the value used in this study. During the experiment, the nutrients were depleted on day twelve. Also, significant aggregation occurred on the twelfth day of the experiment. This fact was used to help find values for the parameters p and q because experimental values were unavailable. Because day twelve was a peak for aggregation, the amount of nutrients on this day was chosen as a measure for the model's sensitivity. It was assumed, in the model, that once the amount of nutrients was less than $10^{-8} \mu M$ they were depleted and at this point the amount of nutrients was set equal to zero.

For the first run in this study the parameters were set to the following numbers: $p=0.9$, $q=0.3$, $D=2.8$, $A=1.93$, $\alpha=0.001$, $fc=0.06$. In this case the nutrients were depleted at the beginning of day twelve (See Table 2). This corresponds with the tank data. The value of α was chosen to be 0.001 because in previous research it had been estimated to be anywhere between 0.0001 and 0.01

Table 2 Sensitivity Study Results							
fc	p	q	α	D	A	Day nutrients were depleted	Amount of nutrients left after 14 days
0.06	0.9	0.3	0.001	2.8	1.93	12.12	0
0.045	0.9	0.3	0.001	2.8	1.93	-	2.38e-8
0.075	0.9	0.3	0.001	2.8	1.93	-	2.09e-7
0.06	0.85	0.3	0.001	2.8	1.93	-	1.79e-8
0.06	0.95	0.3	0.001	2.8	1.93	-	1.09e-7
0.06	0.9	0.225	0.001	2.8	1.93	11.58	0
0.06	0.9	0.375	0.001	2.8	1.93	13.75	0
0.06	0.9	0.3	0.0005	2.8	1.93	-	2.58e-8
0.06	0.9	0.3	0.0015	2.8	1.93	13.0	0
0.06	0.9	0.3	0.001	2.6	1.93	-	1.64e-4
0.06	0.9	0.3	0.001	3.0	1.93	10.5	0
0.06	0.9	0.3	0.001	2.8	1.45	13.37	0
0.06	0.9	0.3	0.001	2.8	2.41	12.58	0

(Ackleh et. al. 1995). The initial number of single cells in the tank experiment is not known exactly but is estimated to be around the value 0.045 per mm^3 . The values of p and q were chosen by fitting the nutrient depletion of the model to that of the tank experiment. The fractal dimension, D , and the proportionality constant, A , were estimated using the least squares method to fit the output of the model to the tank data.

The first parameter changed was f_c , the initial number of free cells. When f_c was decreased by 25%, the nutrients were not depleted at the end of day fourteen. Even though there was a small amount of nutrients left over, this shows a 2 day delay from the first run. When the parameter f_c was increased by 25% a similar result occurred, a two day delay in nutrient depletion.

The second parameter changed was p , the percent of live cells in an aggregate. The model was more sensitive to this parameter than to the parameter f_c . A two day delay occurred with a decrease of only 5.5%. Yet when the parameter p was increased by 5.5% the same result occurred, a two day delay. This was unexpected because one would expect an increase in the number of live cells to decrease the time for nutrient depletion. If $p = 0$, i.e. all cells in the aggregate are dead, then after fourteen days there were two thirds of the nutrients left. This shows that when 90% of the aggregate is alive, the live cells in the aggregate as well as their offspring consumed over two thirds of the nutrients in twelve days.

When the parameter q was decreased by 25%, the nutrients were depleted half way through the eleventh day, only a half a day early. At the same time when q was

increased by 25%, the nutrients depleted three fourths of the way through day 13. This shows that the model is not as sensitive to q as it is to p or f_c . It should be noted that for these runs p was always significantly greater than q . Some runs were done with p smaller, in the .5 range, and in these cases when q was zero there were still nutrients left at the end of the run. This supports the idea that the lower the percent of live cells in aggregates, the higher the percent of new born cells should be free in order to consume the same amount of nutrients. Hence, as p decreases, q needs to decrease to keep nutrient consumption constant.

Increasing the sticking probability, α , by 50% resulted in a delay in nutrient depletion of one day while decreasing by 50% resulted in a two day delay. This implies that the aggregation model is relatively insensitive to the parameter α .

On the other hand, aggregation showed to be sensitive to the fractal dimension. When increased by only 7%, the nutrients were consumed half way through the tenth day. Also, when the fractal dimension was decreased by 7% there were nutrients left over at the end of the fourteen days. This was expected since the fractal dimension plays such a big role in the size of the outer radius. The smaller the fractal dimension the larger the outer radius.

The last parameter considered was the proportionality constant A . The model's sensitivity to this parameter was comparatively low. When the constant was changed by 25%, a delay of a day or less occurred.

The results of the sensitivity study show that aggregation is particularly sensitive to the portion of live cells in aggregates and to the fractal dimension of the

aggregate. This study also shows that aggregation is insensitive to the sticking probability, α , which coincides with the results in Ackleh et. al. 1995.

3.2 Parameter Estimation

The fractal dimension, D , and the proportionality constant, A , were estimated using the least square method of fitting the model output to the data from the tank experiment in Santa Barbara. The least squares code was constrained to consider only values of fractal dimension between 0 and 3 since any value outside of this range would have no realistic application. The code was also constrained to only consider values for the proportionality constant between 0 and 3.5 due to the experimental values reported in Wu and Friedlander 1993.

The model output and the tank data were compared in two different ways. The first was by the mean of the difference of the logarithm of the model output and the logarithm of the data denoted by μ . Thus

$$\mu = \frac{1}{NM} \sum_{i=1}^N \sum_{j=1}^M \left[\log(\phi(t_i, x_i) + 1) - \log(z_{i,j} + 1) \right],$$

where $\phi(t_i, x_i)$ is the model output and $z_{i,j}$ is the tank data. The second method of comparison is by the mean of the absolute difference of the logarithm of the model output and the logarithm of the data denoted by $|\mu|$. Hence,

$$|\mu| = \frac{1}{NM} \sum_{i=1}^N \sum_{j=1}^M \left| \log(\phi(t_i, x_i) + 1) - \log(z_{i,j} + 1) \right|.$$

In these estimates, $N = 16$ and $M = 99$.

The first estimation was done with $\alpha = 0.01$ and with an initial guess of $D = 2$ and $A = 1$. This yielded a fractal dimension of 2.5 with a proportionality constant of 2.3. The mean μ was 2.17 while $|\mu|$ was 2.47. Yet with the initial values of $D = 2.8$ and $A = 0.75$ the results were a fractal dimension of 2.8 and proportionality constant of 1.28 with $\mu = 2.01$ and $|\mu| = 2.41$, a little better from the previous run.

A second set of estimations were done with $\alpha = 0.0001$. With initial values of $D = 2$ and $A = 2$, the results were a fractal dimension of 2.19 and a proportionality constant of 2.36. In this case the mean, μ , was 2.42 and $|\mu|$ was 2.60. Starting with a fractal dimension of 2.8 and a constant of 0.75 yielded a result of $D = 2.8$ and $A = 0.54$ with $\mu = 2.11$ and $|\mu| = 2.46$. This coincides with the previous results that the aggregation model is somewhat insensitive to the parameter alpha.

A final simulation was done estimating the three parameters, D , A , and α . The initial values of $D = 2.0$, $A = 2.0$, and $\alpha = 0.01$ were used. The results were a fractal dimension of 2.1 with a proportionality constant of 1.7 and a sticking probability of $3.23e-6$. The mean, μ , was 2.55 and $|\mu|$ was 2.68.

Chapter 4

Discussion

The results of the parameter estimation show a fractal dimension of about 2.8. This would tend to say that the aggregates are close to three dimensional. This is contrary to the expected result of a fractal dimension between 1 and 2 due to the tendency of diatom cells to form linear chains. One explanation for this higher dimension may be found in the assumption that all aggregates have the same fractal dimension. In reality, aggregates with more cells should have a smaller fractal dimension while aggregates with fewer cells should have a fractal dimension close to if not equal to three. Hence, this assumption could skew the fractal dimension to be higher. Another reason could be that this study only considered aggregates of size less than 1 mm^3 . Thus many larger aggregates with potentially smaller fractal dimension were not included.

The estimation results showed a proportionality constant ranging between 0.5 and 2.36. Although experimental values show this constant to be anywhere from 0 to 3.5, it is most commonly around 1 (Wu and Friedlander 1993). Therefore these results are not unreasonable.

An extension of this aggregation model could be made by introducing a size dependent fractal dimension. This would allow for the smaller size classes to have larger fractal dimension and the large size classes to have smaller fractal dimension.

By including the outer radius, fractal dimension played a role in the settling velocity, contact efficiencies for both shear motion and differential settling, and in the multiplier of the shear and differential coagulation kernels. Further research may include fractal dimension in the model through a medium other than the outer radius.

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Vita

Nicole Puckett was born in upstate New York in 1972. She lived there until she was twelve, when she and her family moved to Mason, Ohio where she graduated from William Mason High School in 1990. Nicole continued her education at Southern College of Seventh-Day Adventists. She graduated in 1994 with a Bachelor of Science degree in Mathematics and certification to teach on the secondary level. In the summer of 1994, she was married to Bryan Scott Puckett and started graduate school at the University of Tennessee in Knoxville. There she received her Masters of Science degree in Mathematics in August 1996.