

HERIOT-WATT UNIVERSITY

**Topics In Coagulation-Fragmentation
Equations**

Matab Alghamdi

November 20, 2014

SUBMITTED FOR THE DEGREE OF
DOCTOR OF PHILOSOPHY IN MATHEMATICS
ON COMPLETION OF RESEARCH IN THE
DEPARTMENT OF MATHEMATICS,
SCHOOL OF MATHEMATICAL AND COMPUTER SCIENCES.

This copy of the thesis has been supplied on the condition that anyone who consults it is understood to recognise that the copyright rests with the author and that no quotation from the thesis and no information derived from it may be published without the written consent of the author or the University (as may be appropriate).

Abstract

In this thesis we study the mathematics of a model for the dynamics of cluster growth. The sizes of the clusters change in time as the clusters undergo coagulation and fragmentation events. The equations are for $j = 1, 2, \dots$

$$c'_j = \frac{1}{2} \sum_{k=1}^{j-1} [a_{j-k,k} c_{j-k} c_k - b_{j-k,k} c_j] - \sum_{k=1}^{\infty} [a_{j,k} c_j c_k - b_{j,k} c_{j+k}] \quad (1.1)$$

where $c_j(t)$ is the concentration of clusters of size j and $a_{j,k}, b_{j,k}$ are the constant rates of coagulation and fragmentation.

Chapter 1 reviews some results on (1.1) and introduces some mathematical tools used in the thesis. It also introduces the concept of gelation, which is the formation of an infinite cluster leading to the loss of mass conservation.

In Chapter 2 we study gelation in (1.1) and discuss finite dimensional approximations which are used for numerical studies. We explain why a certain finite dimensional system which does not conserve density is suitable for numerical studies of (1.1) including gelation.

All solutions of the finite dimensional system converge to zero and Chapter 3 deals with the asymptotic behaviour. For the case in which the coagulation and fragmentation terms are non zero and satisfy a detailed balance condition, we obtain a general result on the asymptotic decay. However, for the pure coagulation case ($b_{j,k} = 0$), we show that a wide variety of asymptotics is possible.

Chapter 4 is concerned with a model for the treatment of Alzheimer's disease. The model is a modified form of (1.1). We prove some mathematical results for the system and obtain an approximate formula for the decay rate.

Chapter 5 deals with numerical approximations to the continuous version of (1.1). We consider a piecewise constant in space approximation in both collocation and the Galerkin formulation. Numerical results indicate that the Galerkin finite element method has second order accuracy. These approximations of the continuous problem are themselves discrete systems like (1.1).

Acknowledgements

All praise be to Allah, the almighty, and peace be upon his slave and last messenger, Mohammad, (PBUH). It gives me a great pleasure to dedicate this achievement to my parents, wife (Huda), kids (Bader, Adil, Batail), my brother Yousif , my sisters (Muna, Amenah and Afrah) and friends.

Special thanks to my supervisor Prof Dugald Duncan who helped in this study through his continuous supervision. I should also express my thanks to my second supervisor Prof Jack Carr for always being there when I needed him.

Contents

1	Background	2
1.1	Introduction	2
1.2	The kinetic coefficients	4
1.3	Exact solutions	6
1.4	Existence and gelation	7
1.5	Background results	10
1.5.1	Centre manifolds	10
1.5.2	Moment inequalities	12
1.6	Outline of thesis	14
2	Coagulation-fragmentation dynamics	18
2.1	Gelation in coagulation equations	18
2.2	Gelation in coagulation-fragmentation equations	22
2.3	Finite dimensional truncations	31
2.4	Numerical results	34
3	Asymptotics for the finite dimensional case	48
3.1	Introduction	48

CONTENTS

3.2	Coagulation-fragmentation dynamics	49
3.3	Becker-Döring equation	50
3.4	The general case with detailed balance	65
3.5	Coagulation dynamics	76
3.6	Constant coagulation rates	78
3.7	The modified system	85
3.8	Analysis of the $n=2$ case.	87
4	A model for the treatment of Alzheimer's disease	108
4.1	Introduction	108
4.2	A modified Becker - Döring equation	110
4.3	Existence and positivity of solution	111
4.4	The equilibrium solution and its stability	114
4.5	Effect of treatment	119
4.6	Estimate of the decay rate	124
5	Numerics of continuous coagulation - fragmentation	135
5.1	Continuous coagulation-fragmentation systems and the Smoluchowski equation	135
5.2	Piecewise constant collocation approximation	139
5.2.1	Numerical results	140
5.3	Galerkin finite element approximation	143
5.3.1	Numerical results	148
6	Concluding remarks	151

List of Figures

2.1	$M_1(t)$ for (2.3.7) with $a_{jk} = jk$, $b_{jk} = 0$ and $n = 100$	35
2.2	$M_1(t)$ for (2.3.7) with $a_{jk} = jk$, $b_{jk} = 0$ and $n = 100$	35
2.3	log – log plot of $M_1(t)$ against t for (2.3.7) with $a_{jk} = jk$, $b_{jk} = 0$ and $n = 100$	36
2.4	$M_2(t)$ for (2.3.7) with $a_{jk} = jk$, $b_{jk} = 0$ and $n = 100$	37
2.5	$M_3(t)$ for (2.3.7) with $a_{jk} = jk$, $b_{jk} = 0$ and $n = 100$	37
2.6	$M_1(t)$ for (2.3.7) with $a_{jk} = (jk)^{3/4}$, $b_{jk} = 0$ and $n = 100$	38
2.7	$M_1(t)$ for (2.3.7) with $a_{jk} = jk$, $b_{jk} = 2$ and $n = 10$	39
2.8	$M_1(t)$ for (2.3.7) with $a_{jk} = jk$, $b_{jk} = 2$ and $n = 10$	40
2.9	$M_1(t)$ for (2.3.7) with $a_{jk} = jk$, $b_{jk} = 2$ and $n = 100$	41
2.10	$M_1(t)$ for (2.3.7) with $a_{jk} = jk$, $b_{jk} = 2$ and $n = 100$	41
2.11	$M_1(t)$ for (2.3.7) with $a_{jk} = jk$, $b_{jk} = 5$ and $n = 10$	42
2.12	$M_1(t)$ for (2.3.7) with $a_{jk} = jk$, $b_{jk} = 5$ and $n = 10$	43
2.13	$M_1(t)$ for (2.3.7) with $a_{jk} = jk$, $b_{jk} = 5$ and $n = 100$	43
2.14	$M_1(t)$ for (2.3.7) with $\alpha = 3$, $b = 1$ in (2.4.2) and $n = 100$	44
2.15	$M_1(t)$ for (2.3.7) with $a_{jk} = jk$, $b_{jk} = \frac{b(j+k)^{\alpha+1}}{(jk)^\alpha}$ when $\alpha = 3$, $b = 0.5$ and $n = 100$	45

LIST OF FIGURES

2.16	$M_1(t)$ for (2.3.7) with $a_{jk} = jk, b_{jk} = \frac{b(j+k)^{\alpha+1}}{(jk)^\alpha}$ when $\alpha = 1,$ $b = 0.6$ and $n = 100.$	46
2.17	$M_1(t)$ for (2.3.7) with $a_{jk} = jk, b_{jk} = \frac{b(j+k)^{\alpha+1}}{(jk)^\alpha}$ when $\alpha = 1,$ $b = 0.2$ and $n = 100.$	47
2.18	$M_2(t)$ for $a_{jk} = jk, b_{jk} = \frac{b(j+k)^{\alpha+1}}{(jk)^\alpha}$ when $\alpha = 1, b = 0.2$ and $n = 100.$	47
3.1	Graph of $M_1(t)$ for $n = 6.$ See Example A.	61
3.2	Graph of $t^{1/n}c_1(t)[(n^2 + n)a_nQ_n]^{1/n}$ for $n = 6.$ See Example A.	62
3.3	Graph of $M_1(t)$ for $n = 10.$ See Example A.	62
3.4	Graph of $M_1(t)$ for $n = 20.$ See Example A.	63
3.5	Graph of $M_1(t).$ See Example B.	64
3.6	Graph of $t^{1/n}c_1(t)[(n^2 + n)a_nQ_n]^{1/n}.$ See Example B.	64
3.7	Graph of $M_1(t)$ for $n = 2.$ See Example C.	74
3.8	Graph of $(nA)^{\frac{1}{n}}t^{1/n}c_1(t)$ for $n = 2.$ See Example C.	74
3.9	Graph of $(nA)^{\frac{1}{n}}t^{1/n}c_1(t)$ for $n = 6.$ See Example C.	75
3.10	Graph of $M_1(t)$ for $n = 6.$ See Example C.	76
3.11	Theorem (3.6.3) when $n = 4$ with different j	85
3.12	Graph of $tc_2(t).$ The initial condition is $c_1(0) = 0.1, c_2(0) = 0.5.$	89
3.13	Behaviour of $\tau y_1(\tau)$ when $\alpha = 0.5 = \beta.$ The initial conditions are $c_1(0) = 0.1, c_2(0) = 0.5.$	92
3.14	Graph of $\tau y_1(\tau)$ when $\alpha = \beta = 1, c_1(0) = 0.1, c_2(0) = 0.5.$	92
3.15	Graph of $t(\ln t)^{1/2}c_1(t)$ when $\alpha = \beta = 1, c_1(0) = 1, c_2(0) = 0.$	93
3.16	Graph of $tc_2(t)$ when $\alpha = \beta = 1, c_1(0) = 1, c_2(0) = 0.$	93
3.17	Regions P, Q and $S.$	99

LIST OF FIGURES

4.1	$A\beta$ burden for steps (a), (b) and (c).	121
4.2	Step B calculation.	123
4.3	Step C calculation.	124
4.4	Rapid decay of $c_1(t)$ in step B.	125
4.5	$F(t)$ for step B.	133
4.6	$F(t)$ for step C.	134
5.1	The comparison of the numerical piecewise approximation and analytical solution for the constant kernel $k(x, y) = 1$ with initial value (5.2.2) at $L = 100$, $N = 1000$ and $t = 1$	141
5.2	The convergence of the piecewise constant collocation approximation using $N = 20, 60, 180, 540$ and $L = 20$ for the constant kernel $k(x, y) = 1$ with initial value (5.2.2) at $t = 1$	142
5.3	The numerical error ϵ_h defined by (5.2.3) using $N = 20, 60, 180, 540, 1620, 4860, 14580$ and $L = 20$ for the constant kernel $k(x, y) = 1$, $k(x, y) = x + y$ and $k(x, y) = xy$ with initial value (5.2.2) at $t = 1$. We see the error estimate appears to converge to 1st order.	143
5.4	The comparison of the numerical Galerkin approximation and analytical solution for the constant kernel $k(x, y) = 1$ with initial value (5.2.2) at $L = 100$, $N = 1000$ and $t = 1$	149
5.5	Computing the numerical error ϵ_h defined in (5.2.3) using $N = 20, 60, 180, 540, 1620, 4860$ and $L = 20$ for the constant kernel $k(x, y) = 1$, $k(x, y) = x + y$ and $k(x, y) = xy$ with initial value (5.2.2) at $t = 1$. We see the error estimates appear to be 2nd order.	150

Chapter 1

Background

1.1 Introduction

Consider a system of a large number of clusters of particles. The particles consist of an integer number of monomers and we can scale the mass so that the mass of the monomer is 1. The mass of a j -cluster consisting of j monomers is then j .

The clusters can coagulate to form larger clusters or fragment to form smaller ones. Let $c_j(t) \geq 0$ be the concentration of clusters of size j . The coagulation-fragmentation equations are for $j = 1, 2, \dots$ [1, 2]

$$c'_j = \frac{1}{2} \sum_{k=1}^{j-1} [a_{j-k,k} c_{j-k} c_k - b_{j-k,k} c_j] - \sum_{k=1}^{\infty} [a_{j,k} c_j c_k - b_{j,k} c_{j+k}], \quad (1.1.1)$$

where a prime denote $\frac{d}{dt}$. We explain the terms in the above equation. The constant $a_{j,k} \geq 0$ is the coagulation coefficient while the constant $b_{j,k} \geq 0$ is the fragmentation coefficient. We assume that $a_{j,k}$ and $b_{j,k}$ are symmetric.

We first describe the coagulation terms. We assume that the rate at which a

$(j - k)$ - cluster merges with a k - cluster is proportional to the concentration $c_{j-k}(t)$ and $c_k(t)$ with $a_{j-k,k}$ the proportionality constant. We assume that the mergers $j - k$ with k and k with $j - k$ are equally likely so that the contribution of the $j - k$ and k merger is

$$\frac{1}{2}a_{j-k,k}c_{j-k}c_k.$$

Summing all these contributions gives the first term in (1.1.1). Also, a cluster of size j can be lost by combining with any other cluster. This is represented by the third term in (1.1.1).

Fragmentation is the process by which a cluster splits into two pieces. The rate at which a $(j + k)$ - cluster splits into a j - cluster and a k - cluster is $b_{j,k}$. The second term in (1.1.1) is a loss of a j - cluster to smaller ones. The final term in (1.1.1) is the contribution of j - clusters from the fragmentation of larger clusters.

Equation (1.1.1) was first derived in [41] for the case in which $b_{j,k} \equiv 0$ and see [13] for the general case. The cluster size could also be taken to be a continuous variable and we consider this case in Chapter 5.

The above equations have been used in many applications. Examples include astrophysics [39], colloidal science [20] and material science [36]. In Chapter 4 we discuss an application to mathematical biology.

The mass of clusters of size j at time t is $jc_j(t)$. The total mass or density of the system is then

$$\rho(t) = \sum_{j=1}^{\infty} jc_j(t). \quad (1.1.2)$$

In the derivation of the model (1.1.1), for each coagulation and fragmentation event the total mass is conserved, so we might expect that $\rho(t)$ is constant. In certain

circumstances however, the density decreases. The mathematical reason is that larger and larger clusters are forming which escape to infinity. Physically this is interpreted as some of the particles being transferred to a new phase. This loss of mass is known as gelation. The question of when gelation occurs depends on the kinetic coefficients $a_{j,k}$ and $b_{j,k}$ as well as the initial data.

1.2 The kinetic coefficients

We first list some special cases of the coagulation-fragmentation equations (1.1.1). The first is pure coagulation in which fragmentation events are neglected so that $b_{j,k} \equiv 0$. This case has been extensively studied especially in the area of gelation. The other extreme case is pure fragmentation in which $a_{j,k} \equiv 0$. Here the equations are linear and are often studied using standard tools from functional analysis. See [28] for some recent work, which also includes coagulation.

The final special case is the Becker-Doring equations. For this system, a j - cluster can only increase or decrease its mass by one unit at a time. Hence $a_{j,k} = b_{j,k} = 0$ if both j and k are greater than 1. This system is a good model for a number of phase transition problems [35]. We study a modified version of this system in Chapter 4.

In his work on the pure coagulation equation, Smoluchowski assumed that $a_{j,k}$ was equal to a constant [41]. In general, the work on coagulation coefficients concentrate on two aspects:

- (a) how a large cluster interacts with a small cluster. Hence we need the behaviour of $a_{j,k}$ for k fixed and $j \rightarrow \infty$.
- (b) how two large clusters interact, that is, how $a_{j,k}$ behaves for $j, k \rightarrow \infty$.

Since the mass of a monomer is 1, the mass of a j - cluster is j and its volume is proportional to j . If the clusters are spheres, then the surface area behaves like $j^{2/3}$ while the diameter behaves like $j^{1/3}$ for large j . If the rate at which clusters merge depends on surface area then we would have $a_{j,k} \sim (jk)^{2/3}$ for large j and k . Similarly, if the dimensions of the diameter are the driving force then $a_{j,k} \sim (jk)^{1/3}$. If the coagulation mechanism depended on the volume then $a_{j,k} \sim jk$. This last case is often used in certain models of polymerisation [24], For a list of some commonly used $a_{j,k}$ see Table 1 in [11].

There is less information available for the fragmentation coefficients. Suppose that surface effects were important and consider a cluster of size $j+k$ with both j and k large. Then we would expect $b_{j,k}$ to be small since this would lead to a large increase in surface area. This idea leads to the concept of weak and strong fragmentation [1] which has implications for density conservation.

For the general case of (1.1.1) it is usually assumed that detailed balance holds:

$$a_{j,k}Q_jQ_k = b_{j,k}Q_{j+k} \tag{1.2.1}$$

for some $Q_j > 0$ [1]. We note that the detailed balance condition always holds for the Becker-Döring equation.

1.3 Exact solutions

In this section we give the exact solution to two cases of the pure coagulation equation.

We use the notation

$$M_p(t) = \sum_{j=1}^{\infty} j^p c_j(t) \quad (1.3.1)$$

for the p th moment of solution.

We begin with $a_{j,k} = jk$, $b_{j,k} = 0$ and initial data $c_j(0) = \delta_{j,1}$. The solution for this case was given in [32]. The equation (1.1.1) takes the form

$$c'_j = \frac{1}{2} \sum_{k=1}^{j-1} (j-k)k c_{j-k} c_k - j M_1(t), \quad (1.3.2)$$

where $M_1(t)$ is given by (1.3.1) with $p = 1$. Equation (1.3.2) can be solved recursively to find $c_j(t)$ in term of $M_1(t)$. An explicit form for $c_j(t)$ is found by using (1.3.1) with $p = 1$. The solution is

$$c_j(t) = \begin{cases} \frac{j^{j-3} t^{j-1} e^{-jt}}{(j-1)!} & 0 \leq t \leq 1, \\ \frac{c_j(1)}{t} & t > 1. \end{cases} \quad (1.3.3)$$

Also,

$$M_1(t) = \begin{cases} 1 & t \leq 1, \\ \frac{1}{t} & t > 1 \end{cases} \quad (1.3.4)$$

and

$$M_2(t) = (1-t)^{-1}. \quad (1.3.5)$$

This shows that there is gelation with $M_1(t)$ constant for $t \leq 1$ and decreasing for $t > 1$. The loss of mass at time $t = 1$ is associated with the formation of an infinite

cluster. Note also that the second moment becomes infinite at the gelation point $t = 1$.

We now consider the case $a_{j,k} = 1$, $b_{j,k} = 0$ with initial data $c_j(0) = \delta_{j,1}$. This case was first derived by Smolochowski and its solution has often been rederived (see for example [17]). The equation is

$$c_j' = \frac{1}{2} \sum_{k=1}^{j-1} c_{j-k} c_k - c_j M_0(t), \quad (1.3.6)$$

and this can be solved recursively to find $c_j(t)$ in terms of $M_0(t)$. The explicit form for $c_j(t)$ is found by using (1.3.1) with $p = 0$. The solution is

$$c_j(t) = \frac{4}{(t+2)^2} \left(\frac{t}{t+2} \right)^{j-1}. \quad (1.3.7)$$

For this case, $M_1(t) = 1$ for all t so that there is no gelation. Since $c_j(t)$ converges exponentially fast as $j \rightarrow \infty$, all of the moments $M_p(t)$ are finite for $p > 0$. In Section 3.6 we derive the solution to a finite dimensional version of (1.3.6).

In general, for the pure coagulation equation we have that for each j , $c_j(t) \rightarrow 0$ as $t \rightarrow \infty$. From (1.3.7) we see that $c_j(t)$ decays like t^{-2} . For the larger coagulation coefficients $a_{j,k} = jk$, from (1.3.3) we have that $c_j(t)$ decays like t^{-1} .

1.4 Existence and gelation

In this section we introduce some of the concepts that have been useful in the study of (1.1.1). We also review some results on existence and gelation.

Consider the finite dimensional system for $c = (c_1, c_2, \dots, c_n)$,

$$c'_j = \frac{1}{2} \sum_{k=1}^{j-1} W_{j-k,k}(c) - \sum_{k=1}^{n-j} W_{jk}(c), \quad (1.4.1)$$

where

$$W_{j,k} = a_{jk}c_jc_k - b_{j,k}c_{j+k}. \quad (1.4.2)$$

It is easy to show that for nonnegative initial data, (1.4.1) has a solution for all $t \geq 0$ which conserves density

$$\sum_{j=1}^n jc_j(t) = \sum_{j=1}^n jc_j(0). \quad (1.4.3)$$

The usual method for proving existence of solutions to (1.1.1) is to prove that as $n \rightarrow \infty$, the solution of (1.4.1) has a limit which satisfies (1.1.1). There has been extensive work on this problem [1, 10, 18, 19, 42]. Solutions exist when $a_{j,k} \leq jk$ for any fragmentation coefficients. If $b_{j,k} = 0$ and $a_{j,k} = r_j + r_k$, $r_j \geq j^\alpha$ with $\alpha > 1$, then there are no solutions to (1.1.1) with nontrivial initial data [6]. We note from [29] that if $b_{j,k} = 0$ and $a_{j,k} = (jk)^\alpha$, $\alpha > 1$ then there are solutions to (1.1.1) of the form

$$c_j = \frac{\alpha_j}{t+1}, \quad (1.4.4)$$

with finite density.

For the pure fragmentation case, there is a large class of fragmentation coefficients (for example, $b_{j,k} = (j+k)^\beta$, $\beta > -1$), for which (1.1.1) has solutions with increasing density [1]. This result was extended in [18] to include coagulation. These spurious

solutions are of no physical interest. Solutions of (1.1.1) which are obtained as limits of finite-dimensional systems such as (1.4.1) are called admissible solutions. For any admissible solution, the density is non-increasing and this excludes the spurious solutions described above. We only consider admissible solutions in this thesis.

We now discuss the issue of gelation, that is, do solutions of (1.1.1) conserve the density (first moment) $\rho(t)$ given by (1.1.2)? We first consider the pure coagulation case with

$$a_{j,k} = (jk)^\alpha.$$

In Section 1.3 we showed that for the initial data $c_j(0) = \delta_{j,1}$, the density was conserved if $\alpha = 0$ and that we had gelation when $\alpha = 1$. In general, if $a_{j,k} \leq (j+k)$ it is shown in [1] that $\rho(t)$ is constant. Hence solutions conserve density for $\alpha \leq 1/2$.

The case

$$\frac{1}{2} < \alpha < 1 \tag{1.4.5}$$

is more difficult. It was proved in [29] that for the case (1.4.5), equation (1.1.1) had a finite density solution of the form (1.4.4). Formal arguments indicated that conservation of density failed for all solutions. Proofs of this were given in [25] using probabilistic arguments and in [19] using differential inequalities. We refer to [19] for the class of coagulation coefficients for which gelation has been proved.

This issue of gelation for the general coagulation-fragmentation equation is complicated. Suppose that for a given $a_{j,k}$ we have gelation when $b_{j,k}$ is zero. If we now take $b_{j,k} \neq 0$ but 'small' compared to $a_{j,k}$ then we again have gelation. However, if the fragmentation is sufficiently strong then solutions will conserve density. The question of gelation can also depend on the density of the initial data. We refer to [18] and

the references there for mathematical results. We discuss some of the issues involved in Chapter 2.

1.5 Background results

In this section we outline some theory which we use in the thesis. The results on centre manifold theory will be used in Sections 3.3, 3.4 and 3.7 while the moment inequalities are used in Sections 2.1 and 2.2.

1.5.1 Centre manifolds

Consider the differential equation

$$x' = f(x), \quad x \in R^m, \quad (1.5.1)$$

with $f(0) = 0$ so that the origin is an equilibrium point. The goal is to study the stability of this equilibrium. The linearised problem is

$$x' = Ax = Df(0)x$$

If the eigenvalues of A all have negative real parts then the equilibrium point $x = 0$ is an asymptotically stable solution of (1.5.1).

Suppose now that that the matrix A has p eigenvalues with real part zero and $m - p$ eigenvalues with negative real parts. We can use centre manifold reduction to reduce the dynamics of (1.5.1) for small x to a p dimensional equation. In particular, this lower dimensional equation determines the stability the of equilibrium $x = 0$ for

(1.5.1).

We will only need $p = 1$ in this thesis so we give the theory just for this case. The summary given below is based on [4].

Consider the system

$$x' = f(x, y), \quad y' = By + g(x, y), \quad (x, y) \in R \times R^n \quad (1.5.2)$$

where all the eigenvalues of the matrix B have negative real parts, the functions f and g are sufficiently smooth and

$$f(0, 0) = 0, \quad Df(0, 0) = 0, \quad g(0, 0) = 0, \quad Dg(0, 0) = 0$$

where Df is the Jacobian matrix of f and similarly for Dg .

We consider first the linear case where f and g are identically zero so that (1.5.2) has the two invariant manifolds $x = 0$ and $y = 0$. The invariant manifold $x = 0$ is called the stable manifold, and on the stable manifold all solutions decay to zero exponentially fast. The invariant manifold $y = 0$ is called the centre manifold. In general, an invariant manifold $y = h(x)$ for (1.5.2) defined for small $|x|$ with $h(0) = 0$ and $Dh(0) = 0$ is called a centre manifold.

The general theory states that there exists a centre manifold $y = h(x)$ for (1.5.2) and that the equation on the centre manifold

$$u' = f(u, h(u)), \quad u \in R^n \quad (1.5.3)$$

determines the dynamics of (1.5.2) near $(x, y) = (0, 0)$. If the zero solution of (1.5.3)

is stable, we can represent small solutions of (1.5.2) as $t \rightarrow \infty$ by

$$x(t) = u(t) + O(e^{-\gamma t}), \quad y(t) = h(u(t)) + O(e^{-\gamma t})$$

where $\gamma > 0$ is a constant.

To use this we need to know enough about the centre manifold $y = h(x)$ in order to determine the local dynamics of (1.5.3). If we substitute $y(t) = h(x(t))$ into the second equation in (1.5.2) we obtain

$$N(h(x)) = h'(x) [Ax + f(x, h(x))] - Bh(x) - g(x, h(x)) = 0. \quad (1.5.4)$$

The general theory tells us that the solution h of (1.5.4) can be approximated by a polynomial in x , that is, if $q \geq 2$ with $N(\phi(x)) = O(|x|^q)$ as $x \rightarrow 0$ then $h(x) = \phi(x) + O(|x|^q)$.

For equations (1.5.2) there is also an n dimensional invariant manifold tangential to the y -axis called the stable manifold. On the stable manifold all solutions decay to zero exponentially fast.

1.5.2 Moment inequalities

For a solution c of the coagulation-fragmentation equations, we formally define the moment $M_\alpha(t)$ by

$$M_\alpha(t) = \sum_{k=1}^{\infty} k^\alpha c_k(t). \quad (1.5.5)$$

In this section, we derive an inequality that is used in comparing moments. We first recall Hölder's inequality for sums.

Theorem 1.5.1. *Let $p > 1$ be a real number and define $q > 1$ by*

$$q = \frac{p}{p-1}, \tag{1.5.6}$$

so that

$$\frac{1}{p} + \frac{1}{q} = 1.$$

Suppose that

$$\sum_{k=1}^{\infty} |x_k|^p < \infty \quad \text{and} \quad \sum_{k=1}^{\infty} |y_k|^q < \infty.$$

Then

$$\sum_{k=1}^{\infty} |x_k y_k| \leq \left(\sum_{k=1}^{\infty} |x_k|^p \right)^{\frac{1}{p}} \left(\sum_{k=1}^{\infty} |y_k|^q \right)^{\frac{1}{q}}.$$

The next result is well known, we give a proof for completeness.

Theorem 1.5.2. *Let $0 \leq \alpha < \beta < \gamma$ and suppose that*

$$M_\gamma = \sum_{k=1}^{\infty} k^\gamma c_k < \infty,$$

where $c_k \geq 0$ for all k . Then

$$(M_\beta)^{\gamma-\alpha} \leq (M_\alpha)^{\gamma-\beta} (M_\gamma)^{\beta-\alpha}.$$

Proof: We have that

$$\beta = \frac{\alpha(\gamma - \beta)}{\gamma - \alpha} + \frac{\gamma(\beta - \alpha)}{\gamma - \alpha},$$

so that

$$k^\beta c_k = (k^\alpha c_k)^{\frac{\gamma-\beta}{\gamma-\alpha}} (k^\gamma c_k)^{\frac{\beta-\alpha}{\gamma-\alpha}}.$$

Define p by

$$p = \frac{\gamma - \alpha}{\gamma - \beta} = 1 + \frac{\beta - \alpha}{\gamma - \beta} > 1.$$

From (1.5.6)

$$q = \frac{p}{p-1} = \left(\frac{\gamma - \alpha}{\gamma - \beta} \right) \left(\frac{\gamma - \beta}{\beta - \alpha} \right) = \frac{\gamma - \alpha}{\beta - \alpha}.$$

Let

$$x_k = (k^\alpha c_k)^{\frac{\gamma-\beta}{\gamma-\alpha}} \quad , \quad y_k = (k^\gamma c_k)^{\frac{\beta-\alpha}{\gamma-\alpha}} \quad ,$$

so that

$$x_k^p = k^\alpha c_k \quad , \quad y_k^q = k^\gamma c_k.$$

The result now follows by applying Hölder's inequality.

As an example, taking $\alpha = 0, \beta = 1$ and $\gamma = 2$ in Theorem 1.5.2,

$$M_1^2 \leq M_2 M_0.$$

1.6 Outline of thesis

In Chapter 2 we discuss the occurrence of gelation in the coagulation - fragmentation equations. Numerical methods for these equations are usually based on finite dimensional approximations such as (1.4.1). Since density is conserved for solutions of (1.4.1), this approximation is not much use in studying gelation. Instead we study

the finite dimensional system

$$c_j' = \frac{1}{2} \sum_{k=1}^{n-j} W_{j-k,k} - \sum_{k=1}^{n-j} W_{jk} - \sum_{k=n-j+1}^n a_{j,k} c_j c_k \quad (1.6.1)$$

for $1 \leq j \leq n$, where $W_{j,k}$ is given by (1.4.2). This approximation is given by [3] for the continuous case. For solutions of (1.6.1), the density decreases.

In Chapter 2 we use formal calculations to investigate gelation in a number of examples. Most of these examples have been discussed in the literature although Example 2 in Section 2.2 is new. We present some numerical examples based on the approximation (1.6.1). Among other things, the results show that the method is well suited to the detection of the gelation phenomenon.

The only mathematical study of (1.6.1) is for the pure coagulation case $a_{j,k} = r_j r_k$ [11]. For this case, as well as the general case, all solutions converge to zero. Chapter 3 is a study of the details of this convergence.

When the detailed balance condition (1.2.1) holds, the infinite system (1.1.1) has equilibrium solutions of the form

$$c_j = Q_j z^j, \quad j = 1, 2, \dots \quad (1.6.2)$$

with density

$$\sum_{j=1}^{\infty} j Q_j z^j \quad (1.6.3)$$

as long as (1.6.3) is finite [2]. The only equilibrium solution to the finite dimensional problem (1.6.1) is the zero solution. All solutions of (1.6.1) converge to zero as $t \rightarrow \infty$.

However, numerical studies show that for solutions of (1.6.1), the density

$$\rho(t) = \sum_{j=1}^n j c_j(t)$$

decays very slowly. In fact, solutions seem to look like the equilibrium solutions (1.6.2). For small initial densities, we prove that for solutions of (1.6.1),

$$c_j(t) \approx Q_j(u(t))^j, \quad 1 \leq j \leq n \quad (1.6.4)$$

where

$$u(t) \approx A t^{-1/n} \quad (1.6.5)$$

with A a positive constant. Since the decay of (1.6.5) is very slow, this explains the slow behaviour. We also present some numerical solutions to support the above asymptotic results. The study of (1.6.1) when the detailed balance condition holds is given in Sections 3.2 - 3.4.

The rest of Chapter 3 studies the pure coagulation case

$$c_j' = \frac{1}{2} \sum_{k=1}^{j-1} a_{j-k,k} c_{j-k} c_k - c_j \sum_{k=1}^n a_{j,k} c_j c_k. \quad (1.6.6)$$

Unlike the case of detailed balance, we show that the asymptotics here is much more complicated and there are no general results. An outline of this work is given in Section 3.5.

In Chapter 4 we study a model for the treatment of Alzheimer's disease. The model was introduced in [8], [9] and has the form of a modified Becker - Doring equation.

The work in [8], [9] only considered numerical results, we prove some mathematical results for the system. The parameters in the model are related to chemical time scales and are measured in fractions of a second so they are small. The time scales involved in the application of the model are very long, and are measured in months and years. We derive an approximation which gives a formula for the decay rate in terms of the parameters.

Finally, in Chapter 5 we consider numerical approximations to the continuous version of the coagulation equations. These approximations are themselves discrete coagulation equations. We first consider a piecewise constant collocation in space approximation. We numerically solve the equation for the three coagulation coefficients,

$$K(x, y) = 1, x + y \text{ and } xy$$

for which exact solutions are available. We then use the Galerkin finite element approximation in an attempt to get more accurate results. Our numerical results using this method for the above coagulation kernels show that it has second order accuracy.

Chapter 2

Coagulation-fragmentation dynamics

2.1 Gelation in coagulation equations

In this section we study the coagulation equation when $b_{j,k} = 0$, see equation (1.1.1)

$$c'_j = \frac{1}{2} \sum_{k=1}^{j-1} a_{j-k,k} c_{j-k} c_k - c_j \sum_{k=1}^{\infty} a_{j,k} c_k. \quad (2.1.1)$$

The following identity is useful for deriving properties of solutions.

Lemma 2.1.1. *Let c be a solution of (2.1.1) and let (g_j) be a sequence. Then*

$$\sum_{j=1}^n g_j c'_j = \frac{1}{2} \sum_R (g_{j+k} - g_j - g_k) a_{jk} c_j c_k - \sum_{j=1}^n g_j \sum_{k=n-j+1}^{\infty} a_{jk} c_j c_k, \quad (2.1.2)$$

where R is the region

$$R = \{(j, k) : j + k \leq n\}.$$

Proof: We multiply each term in (2.1.1) by g_j and sum over j . The first sum is

$$\frac{1}{2} \sum_{j=1}^n g_j \sum_{k=1}^{j-1} a_{j-k,k} c_{j-k} c_k. \quad (2.1.3)$$

The region in (j, k) space over which we are summing in (2.1.3) is R so we can write this as

$$\frac{1}{2} \sum_R g_{j+k} a_{jk} c_j c_k.$$

The second sum is

$$- \sum_{j=1}^n g_j \sum_{k=1}^{\infty} a_{jk} c_j c_k,$$

which may be written as

$$- \left(\sum_R + \sum_{j=1}^n \sum_{k=n-j+1}^{\infty} \right) g_j a_{jk} c_j c_k.$$

Using the symmetry of a_{jk} , we can write the sum over R as

$$- \frac{1}{2} \sum_k (g_j + g_k) a_{jk} c_j c_k,$$

and this completes the proof.

For a solution c of (2.1.1) we can compute the density by

$$M_1(t) = \sum_{j=1}^{\infty} j c_j(t).$$

Putting $g_j = j$ in Lemma 2.1.1 we obtain

$$\sum_{j=1}^n j c_j' = - \sum_{j=1}^n \sum_{k=n-j+1}^{\infty} j a_{jk} c_j c_k. \quad (2.1.4)$$

Letting $n \rightarrow \infty$ in (2.1.4)

$$M_1(t) = M_1(0) - \lim_{n \rightarrow \infty} \int_0^t \sum_{j=1}^n \sum_{k=n-j+1}^{\infty} j a_{jk} c_j(s) c_k(s) ds. \quad (2.1.5)$$

It follows that a solution c conserves density if and only if

$$\lim_{n \rightarrow \infty} \int_0^t \sum_{j=1}^n \sum_{k=n-j+1}^{\infty} j a_{jk} c_j(s) c_k(s) ds = 0. \quad (2.1.6)$$

When the density decreases this is known as gelation. In Chapter 1 we saw that for $a_{jk} = jk$ and $c_j(0) = \delta_{j,1}$, the solution c had the density

$$M_1(t) = \begin{cases} 1 & t \leq 1, \\ t^{-1} & t > 1. \end{cases}$$

In general, it is physically important and a mathematically difficult question to determine if $M_1(t)$ is constant.

To gain insight into this issue we proceed formally. Define the moments M_p by

$$M_p(t) = \sum_{j=1}^{\infty} j^p c_j(t).$$

Letting $g_j = j^p$ in Lemma 2.1.1, taking $n \rightarrow \infty$ and assuming that all the series

converge we obtain

$$\frac{dM_p}{dt} = \frac{1}{2} \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} [(i+j)^p - i^p - j^p] a_{ij} c_i c_j. \quad (2.1.7)$$

Suppose first that $a_{jk} = jk$ and that $M_1(0) = 1$. Assuming density is conserved,

$$\frac{dM_0}{dt} = -\frac{1}{2}. \quad (2.1.8)$$

and

$$\frac{dM_2}{dt} = M_2^2. \quad (2.1.9)$$

From (2.1.8),

$$M_0(t) = M_0(0) - \frac{t}{2},$$

which is negative for $t > 2M_0(0)$. This is impossible so the assumption that density was conserved for all t must be false. This gives a formal proof of gelation for $a_{jk} = jk$.

From (2.1.9),

$$M_2(t) = (M_2^{-1}(0) - t)^{-1},$$

which becomes infinite for finite t giving another formal proof of gelation.

We can use a similar idea to study the gelation problem for the case

$$a_{jk} = \frac{j^\alpha k^\beta + j^\beta k^\alpha}{2}, \quad (2.1.10)$$

with $0 \leq \alpha \leq \beta \leq 1$. From (2.1.7)

$$M_2' = M_{1+\alpha}(t)M_{1+\beta}(t). \quad (2.1.11)$$

Suppose that $M_2(0)$ is finite. Then $M_2' \leq M_2^2$ so that $M_2(t)$ will be finite for small t .

From Theorem 1.5.2 in Chapter 1,

$$M_{1+\alpha} \leq M_1^{1-\alpha} M_2^\alpha, \quad M_{1+\beta} \leq M_1^{1-\beta} M_2^\beta.$$

Hence if in addition to $M_2(0) < \infty$ we have that $\alpha + \beta \leq 1$, from (2.1.11)

$$M_2'(t) \leq M_1^{1-\alpha}(t) M_2^\alpha(t) M_1^{1-\beta}(t) M_2^\beta(t) \leq M_1(0) M_2(t),$$

which shows that $M_2(t) < \infty$ for all t .

However, if $\alpha + \beta > 1$ then it was conjectured that except for the zero solution, density conservation did not hold for all t . This conjecture was based on the existence of explicit gelling solutions of the form $c_j(t) = m_j(t + c)^{-1}$ [29]. The rigorous proofs of gelation which covered cases such as (2.1.10) with $\alpha + \beta > 1$ were given in [25] using probability arguments and [19] which used differential equations methods.

2.2 Gelation in coagulation-fragmentation equations

We study

$$c_j' = \frac{1}{2} \sum_{k=1}^{j-1} W_{j-k,k} - \sum_{k=1}^{\infty} W_{jk}, \quad (2.2.1)$$

with $W_{jk} = a_{jk}c_jc_k - b_{jk}c_{j+k}$. Fragmentation acts in the opposite way from coagulation by splitting a cluster of size $i + j$ into two smaller pieces of size i and j . We would expect fragmentation to inhibit the formation of large clusters and perhaps to even prevent the occurrence of gelation for solutions of (2.2.1).

Unfortunately (2.2.1) can have solutions which are not physical. For the case of

pure fragmentation

$$a_{jk} = 0, \quad b_{jk} = (j+k)^\beta, \quad \beta > -1,$$

it was shown in [1] that for any $\lambda > 0$, (2.2.1) had solutions with density $e^{\lambda t}$. Results of this kind were proved for (2.2.1) in general, that is, under certain conditions on a_{jk} and b_{jk} , there were solutions with $M_1(t) > M_1(0)$ for all $t > 0$.

In order to exclude solutions of this type we need to be more careful about the meaning of a solution. Existence of solutions to (2.2.1) is usually proved by taking a finite dimensional approximation to the equations (see the next section). Solutions are then proved to exist for the infinite system by letting the size of the finite system tend to infinity. The solutions obtained in this way are called admissible and exclude the nonphysical solutions described above. In this section we will proceed formally but we will always be considering admissible solutions.

We will make use of the following identity which is proved in the same way as Lemma 2.1.1 in the previous section:

$$\sum_{j=1}^n g_j c'_j = \frac{1}{2} \sum_R (g_{j+k} - g_j - g_k) W_{jk} - \sum_{j=1}^n g_j \sum_{k=n-j+1}^{\infty} W_{jk}. \quad (2.2.2)$$

$$R = \{(j, k) : j + k \leq n\}.$$

Letting $n \rightarrow \infty$ in (2.2.2) gives

$$\sum_{j=1}^{\infty} g_j c'_j = \frac{1}{2} \sum_{j,k=1}^{\infty} (g_{j+k} - g_j - g_k) W_{jk}. \quad (2.2.3)$$

At the end of this section we give two examples which show that if fragmentation is

strong enough with respect to the coagulation then gelation cannot occur. There is an interplay between the fragmentation size and the total density $M_1(0)$. To demonstrate this we scale the solution of (2.2.1). In order to compare the strength of fragmentation we write

$$b_{jk} = bB_{jk},$$

where $b > 0$ is a constant. Let

$$\bar{c}_j(\tau) = \lambda c_j(t), \quad t = \lambda\tau.$$

Then

$$\frac{d\bar{c}_j(\tau)}{d\tau} = \lambda^2 \frac{dc_j(t)}{dt}.$$

From (2.2.1),

$$\begin{aligned} \frac{d}{d\tau} \bar{c}_j(\tau) &= \frac{1}{2} \sum_{k=1}^{j-1} \lambda^2 W_{j-k,k}(c(t)) - \sum_{k=1}^{\infty} \lambda^2 W_{j,k}(c(t)) \\ &= \frac{1}{2} \sum_{k=1}^{j-1} \bar{W}_{j-k,k}(\bar{c}(\tau)) - \sum_{k=1}^{\infty} \bar{W}_{j,k}(\bar{c}(\tau)), \end{aligned}$$

where

$$\bar{W}_{j,k}(\bar{c}(\tau)) = a_{jk} \bar{c}_j \bar{c}_k - \lambda b B_{jk} \bar{c}_{j+k}.$$

Writing $\bar{M}_1(0)$ for the first moment of the scaled system, we have that $\bar{M}_1(0) = \lambda M_1(0)$.

Suppose we have a result about the absence of gelation which required $M_1(0) = 1$

and b large. Taking $\lambda = b^{-1}$, the scaled system shows that we obtain the same result for fixed fragmentation and small first moment. Similarly, suppose we have a result that says that gelation occurs for fixed fragmentation and large first moment. Taking $\lambda = b^{-1}$, we have a corresponding result for fixed first moment and very small fragmentation.

Example 1. We study the role of fragmentation in the special case

$$a_{jk} = jk, \quad b_{jk} = b \geq 0. \quad (2.2.4)$$

If $b = 0$, we showed in the previous section that any nonzero solution will not conserve density for all t . We want to see if fragmentation with $b > 0$ can prevent gelation.

Lemma 2.2.1.

$$M_0' = -\frac{M_1^2}{2} + \frac{b}{2}(M_1 - M_0). \quad (2.2.5)$$

Proof: From (2.2.3)

$$M_0' = -\frac{1}{2} \sum_{j,k} W_{jk} = -\frac{1}{2} \sum_{j,k} (jk c_j c_k - b c_{j+k}).$$

Summing over the diagonal,

$$\sum_{j,k=1}^{\infty} c_{j+k} = \sum_{r=2}^{\infty} \sum_{k=1}^{r-1} c_r = \sum_{r=2}^{\infty} (r-1) c_r = M_1 - M_0.$$

Also,

$$\sum_{j,k} jk c_j c_k = \left(\sum_{j=1}^{\infty} j c_j \right)^2 = M_1^2.$$

Using the above calculations, the result follows.

The next result shows that if the initial data are large compared with the strength of the fragmentation then we still have gelation.

Theorem 2.2.2. *Suppose that $M_1(0) > b$. Then we cannot have $M_1(t) = M_1(0)$ for all $t > 0$. If $[0, t_g]$ is the largest interval I for which*

$$M_1(t) = M_1(0), \quad t \in I,$$

then

$$t_g < 2b^{-1} \ln(1 - M_0(0)\alpha^{-1}), \quad (2.2.6)$$

where

$$\alpha = b^{-1}M_1(0)(b - M_1(0)).$$

Proof: Suppose $M_1(t) = M_1(0)$ for $t \leq T$. From (2.2.5), for $t \leq T$

$$\frac{d}{dt}(M_0(t)e^{\frac{b}{2}t}) = \left(\frac{M_1(0)}{2} (b - M_1(0)) \right) e^{\frac{b}{2}t} = Ke^{\frac{b}{2}t} < 0. \quad (2.2.7)$$

From (2.2.7), $M_0(\bar{t}) = 0$ for some $\bar{t} > 0$. This shows that we must have $T < \infty$ so that we always have gelation.

The solution of (2.2.7) for $t < T$ is

$$M_0(t)e^{\frac{b}{2}t} = 2b^{-1}Ke^{\frac{b}{2}t} + M_0(0) - 2b^{-1}K$$

so that $M_0(\bar{t}) = 0$ if

$$e^{\frac{b}{2}\bar{t}} = 1 - \frac{M_0(0)}{2b^{-1}K} = 1 - M_0(0)\alpha^{-1},$$

and the result follows.

We now do a formal calculation which indicate how large b should be relative to $M_1(0)$ in order to prevent gelation.

Lemma 2.2.3. *Suppose that $M_3(t) < \infty$. Then*

$$M_2'(t) = M_2^2(t) - \frac{b}{6}M_3(t) + \frac{b}{6}M_1(t). \quad (2.2.8)$$

Proof: From (2.2.3),

$$M_2' = \sum_{j,k} jkW_{jk} = M_2^2 - b \sum_{j,k} jkC_{j+k}. \quad (2.2.9)$$

Summing along the diagonal $j + k = r$, we have that

$$\sum_{j,k} jkC_{j+k} = \sum_{r=2}^{\infty} u_r C_r \quad (2.2.10)$$

$$u_r = \sum_{j=1}^{r-1} j(r-j).$$

By standard results

$$\sum_{j=1}^{r-1} j = \frac{r(r-1)}{2}, \quad \sum_{j=1}^{r-1} j^2 = \frac{r(r-1)(2r-1)}{6},$$

so that

$$u_r = \frac{r^3 - r}{6}.$$

Using this in (2.2.10) gives the result.

Suppose that $M_1(t) = M_1(0)$ for $0 \leq t \leq T$. From Theorem 1.5.2 in Chapter 1,

$M_2^2(t) \leq M_1(t)M_3(t) \leq M_1(0)M_3(t)$ for $T \geq t$. Then for $T \geq t$,

$$M_2' \leq \frac{M_2^2(t)}{6M_1(0)}(6M_1(0) - b) + \frac{b}{6}M_1(0). \quad (2.2.11)$$

If $b \geq 6M_1(0)$ then $M_2(t)$ is bounded on the interval $[0, T]$. This bound on the second moment may be used to estimate the right hand side of (2.2.2) and to show that it converges to zero as $n \rightarrow \infty$. Although this is formal, a rigorous version can be proved for this and similar examples.

In summary, suppose $M_1(0) = 1$. Then for this example we expect gelation if b is small while density should be conserved if b is large.

Example 2. For this example we study a case in which rate coefficients satisfy the detailed balance condition

$$a_{jk}Q_jQ_k = b_{jk}Q_{j+k}, \quad j, k \geq 1, \quad (2.2.12)$$

with $Q_1 = 1$. We consider the family of examples

$$a_{jk} = jk, \quad b_{jk} = \frac{b(j+k)^{\alpha+1}}{(jk)^\alpha}. \quad (2.2.13)$$

This satisfies the detailed balance condition with

$$Q_j = b^{1-j}j^{-(\alpha+1)}.$$

As in the previous example we have gelation if $b = 0$.

Fix $b > 0$ and $\alpha > 1$. We use the same idea as in Theorem (2.2.2) to show that we have gelation for $M_1(0)$ large enough. Suppose $M_1(t) = M_1(0)$ for $t \leq T$. From (2.2.3) for $t \leq T$

$$M_0'(t) = -\frac{M_1^2(0)}{2} + \frac{1}{2} \sum_{j,k} b_{jk} c_{j+k}. \quad (2.2.14)$$

Since $\alpha > 1$ the series

$$\sum_{j,k} b_{jk} c_{j+k} = \sum_{r=2}^{\infty} u_r c_r$$

where

$$u_r = br^{\alpha+1} \sum_{j=1}^{r-1} (j(r-j))^{-\alpha}. \quad (2.2.15)$$

Suppose that we can show that u_r is less than a constant multiple of r . From (2.2.14)

$$M_0'(t) \leq -\frac{M_1^2(0)}{2} + pM_1(0), \quad (2.2.16)$$

for some constant $p > 0$. For large enough $M_1(0)$ the right hand side of (2.2.16) is negative so that $M_0(\bar{t}) = 0$ for some $\bar{t} > 0$. This would show that we have gelation.

We now prove the bound on u_r . By symmetry

$$\sum_{j=1}^{r-1} (j(r-j))^{-\alpha} = 2 \sum_{j=1}^{\lfloor r/2 \rfloor} j^{-\alpha} (r-j)^{-\alpha}, \quad (2.2.17)$$

where $\lfloor r/2 \rfloor$ is the smallest integer greater than (or equal) to $r/2$. Also, for $1 \leq j \leq \lfloor r/2 \rfloor$,

$$(r-j)^{-\alpha} \leq (\text{constant})r^{-\alpha}.$$

Since $\alpha > 1$ the series

$$\sum_{j=1}^{\infty} j^{-\alpha},$$

is convergent. It follows that the series in (2.2.17) is bounded by a constant multiple of $r^{-\alpha}$ so from (2.2.15) we have

$$u_r \leq (\text{constant})r$$

as required. This shows that we have gelation if $\alpha > 1$.

Suppose now that $\alpha \leq 1$ and that $M_1(0)$ is fixed. We give a formal proof that if b is large enough, gelation cannot occur. As in Example 1, the idea is to show that $M_2(t)$ is bounded.

From (2.2.9),

$$M_2' = M_2^2 - b \sum_{j,k} (jk)^{1-\alpha} (j+k)^{\alpha+1} c_{j+k}. \quad (2.2.18)$$

Summing along the diagonal $j+k=r$, the sum of the fragmentation terms is

$$\begin{aligned} & \sum_{r=2}^{\infty} u_r c_r \\ u_r &= r^{\alpha+1} \sum_{j=1}^{r-1} j^{1-\alpha} (r-j)^{1-\alpha}. \end{aligned} \quad (2.2.19)$$

We show that u_r is larger than a constant multiple of r^3 . By symmetry

$$\sum_{j=1}^{r-1} j^{1-\alpha} (r-j)^{1-\alpha} \geq \sum_{j=1}^{\lfloor r/2 \rfloor} j^{1-\alpha} (r-j)^{1-\alpha},$$

where $[r/2]$ is now the biggest integer less than or equal to $r/2$. It follows that

$$\sum_{j=1}^{r-1} j^{1-\alpha} (r-j)^{1-\alpha} \geq k_1, \quad r^{1-\alpha} \sum_{j=1}^{[r/2]} j^{1-\alpha} \geq k_2 r^{3-2\alpha},$$

where K_1, K_2 are positive constants. Using this information in (2.2.19) shows that $u_r \geq kr^{4-\alpha}$ for some $k > 0$. Since $4 - \alpha \geq 3$ it follows that

$$M_2' \leq M_2^2 - bkM_3 + bkM_1. \quad (2.2.20)$$

Suppose now that $M_1(t) = M_1(0)$ for $t \leq T$. Using the inequality $M_2^2 \leq M_1M_3$, for $t \leq T$

$$M_2'(t) \leq M_2^2(t) - bkM_1^{-1}(0)M_2^2(t) + bkM_1(0)$$

so that $M_2(t)$ is bounded on the interval $[0, T]$, if $b \geq k^{-1}M_1(0)$.

2.3 Finite dimensional truncations

In order to develop a numerical scheme for solving coagulation-fragmentation equations of the form (2.2.1) we need to have a maximum size n for clusters. A natural way to do this is to solve the truncated system

$$c_j' = \frac{1}{2} \sum_{k=1}^{j-1} W_{j-k,k} - \sum_{k=1}^{n-j} W_{jk} \quad j = 1, 2, \dots, n. \quad (2.3.1)$$

The above system is often used for mathematical studies of (2.2.1). For example, existence of solutions to (2.2.1) are proved by solving (2.3.1) and letting $n \rightarrow \infty$.

The finite system (2.3.1) is called the maximal n -truncation [11] since $a_{jk} = 0$

for the maximum number of terms. Solving (2.3.1) is a reasonable method for approximating solutions to the infinite system in certain cases. However, for (2.3.1) the density

$$\rho(t) = \sum_{r=1}^n r c_r(t), \quad (2.3.2)$$

is a constant. This is not a useful property if we are studying gelation.

To motivate the truncation used for numerical studies (2.2.1) we first consider the pure coagulation case. The minimal n -truncation is

$$c_j' = \frac{1}{2} \sum_{k=1}^{j-1} a_{j-k,k} c_{j-k} c_k - c_j \sum_{k=1}^n a_{jk} c_k, \quad (2.3.3)$$

for $j = 1, 2, \dots, n$.

It is called minimal since $a_{jk} = 0$ for the least number of terms. This truncation allows for example the interaction



As the truncated density (2.3.2) does not include clusters of size $n + 1$, it is clear that the density should decrease in time. A calculation shows that

$$\rho'(t) = - \sum_{j=1}^n \sum_{k=n-j+1}^n j a_{jk} c_j c_k \leq 0, \quad (2.3.4)$$

confirming this. This is the property we require to mimic gelling solutions in the infinite system.

We now consider the truncation of the fragmentation term. Suppose we use the same idea as in the minimal- n truncation for the coagulation equation. The system would then be

$$c'_j = \frac{1}{2} \sum_{k=1}^{j-1} W_{j-k,k} - \sum_{k=1}^n W_{jk} \quad j = 1, 2, \dots, n. \quad (2.3.5)$$

For this set of equations

$$\rho'(t) = - \sum_{j=1}^n \sum_{k=n-j+1}^n j(b_{jk}c_{j+k} - a_{jk}c_jc_k). \quad (2.3.6)$$

In (2.3.6) the contribution of the fragmentation terms is positive and linear while the coagulation terms are negative and quadratic. It would be very difficult to detect from (2.3.6), either via theory or numerically, if there was an indication of gelation for the infinite system.

The scheme used in [3] is to take the minimal truncation for coagulation and the maximal truncation for fragmentation. The resulting finite dimensional system is

$$c'_j = \frac{1}{2} \sum_{k=1}^{j-1} W_{j-k,k} - \sum_{k=1}^{n-j} W_{jk} - \sum_{k=n-j+1}^n a_{jk}c_jc_k, \quad (2.3.7)$$

for $j = 1, 2, \dots, n$. For (2.3.7) we have that (2.3.4) again holds, i.e.

$$\rho'(t) = - \sum_{j=1}^n \sum_{k=n-j+1}^n ja_{jk}c_jc_k, \quad (2.3.8)$$

which allows for the detection of gelation.

2.4 Numerical results

In this section we present some numerical results for various examples. In all cases we use the finite dimensional approximation given by (2.3.7). Also, for initial data we always take $c_1(0) = 1$, $c_j(0) = 0$ for $j \geq 2$ so that $M_1(0) = 1$. We begin by studying pure coagulation models.

Examples A

We begin with $a_{jk} = (jk)^\alpha$, $b_{jk} = 0$. From Section 2.1 the infinite set of equations exhibit gelation if $\alpha > 1/2$, while the density $M_1(t)$ is conserved if $\alpha \leq 1/2$. For all of our numerical results we take $n = 100$ in (2.3.7) and use the matlab variable step ODE solver ode45 with relative tolerance = 10^{-6} and absolute tolerance = 10^{-20} for the smaller problems. For the larger problems ode15s was used with the same setting and it was allowed to estimate the Jacobian matrix by its own internal process.

Example A1 Let $\alpha = 1$ so that $a_{jk} = jk$. From Section 2.1, the solution to the infinite set of equations satisfies

$$M_1(t) = \begin{cases} 1 & t \leq 1, \\ t^{-1} & t > 1. \end{cases} \quad (2.4.1)$$

Also, the second moment $M_2(t)$ satisfies $M_2(t) = (1 - t)^{-1}$.

Figure 2.1 shows a sharp decrease in $M_1(t)$ at approximately $t = 1$. Also, $M_1(t)$ shows approximately the same rate of decay as that in (2.4.1). Figure 2.2 shows that this decay of $M_1(t)$ continues for larger times. Figure 2.4 shows $M_2(t)$ while Figure 2.5 shows $M_3(t)$.

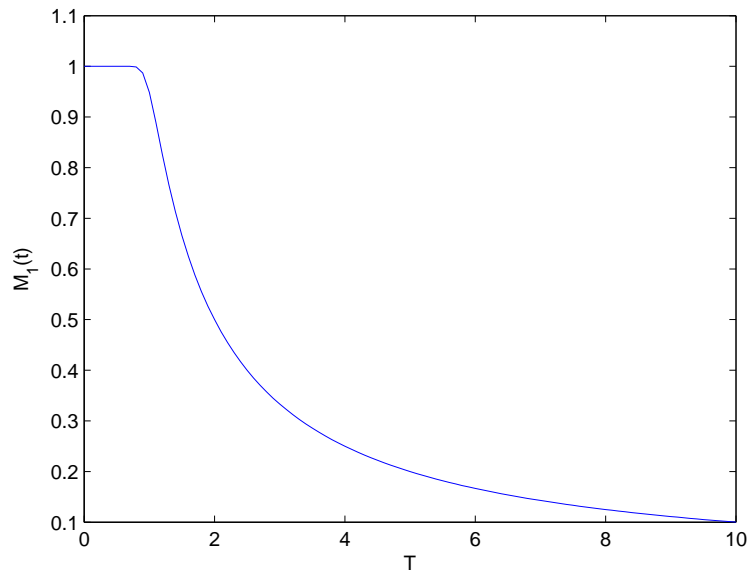


Figure 2.1: $M_1(t)$ for (2.3.7) with $a_{jk} = jk$, $b_{jk} = 0$ and $n = 100$.

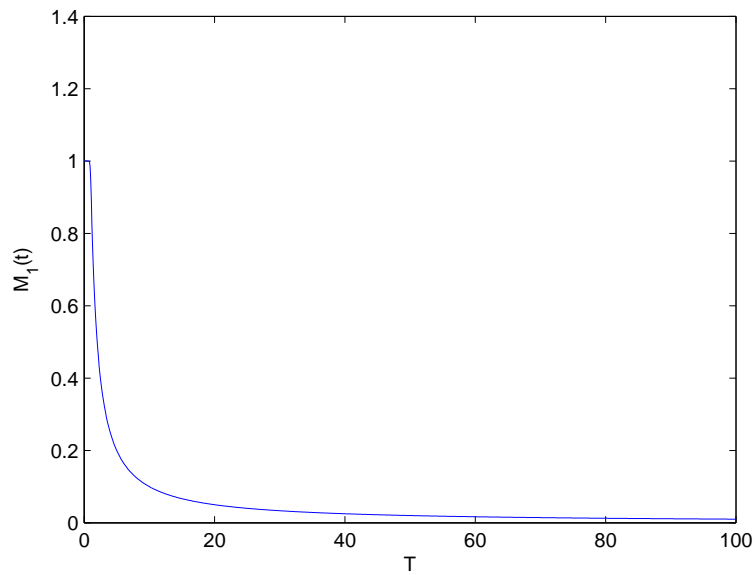


Figure 2.2: $M_1(t)$ for (2.3.7) with $a_{jk} = jk$, $b_{jk} = 0$ and $n = 100$.

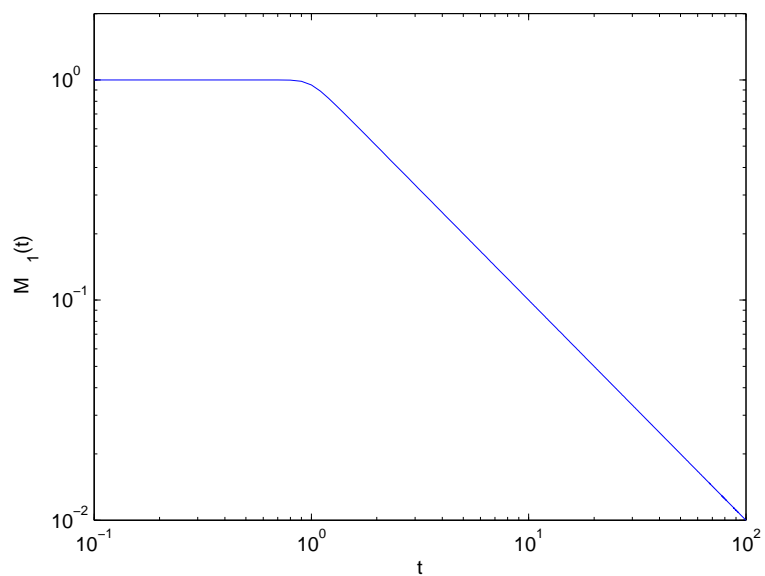


Figure 2.3: log – log plot of $M_1(t)$ against t for (2.3.7) with $a_{jk} = jk$, $b_{jk} = 0$ and $n = 100$.

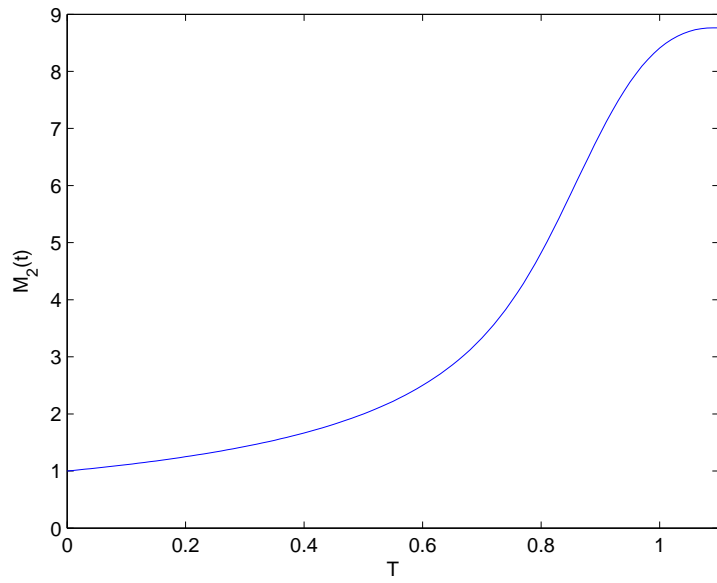


Figure 2.4: $M_2(t)$ for (2.3.7) with $a_{jk} = jk$, $b_{jk} = 0$ and $n = 100$.

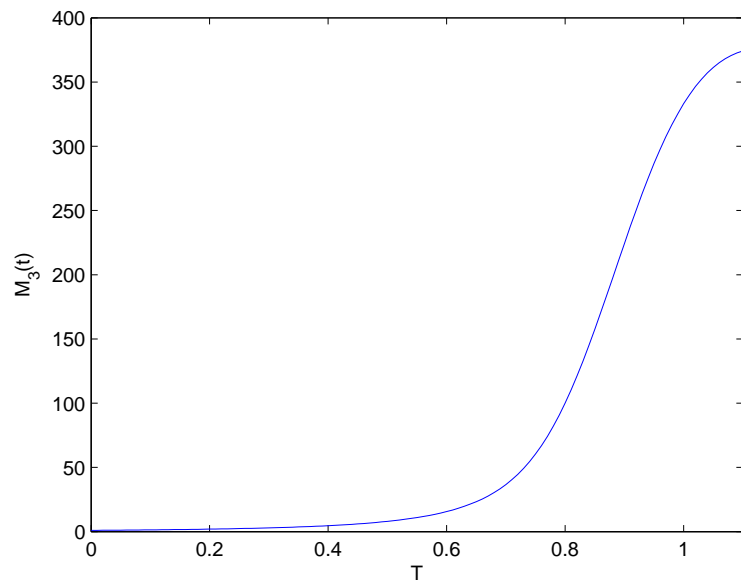


Figure 2.5: $M_3(t)$ for (2.3.7) with $a_{jk} = jk$, $b_{jk} = 0$ and $n = 100$.

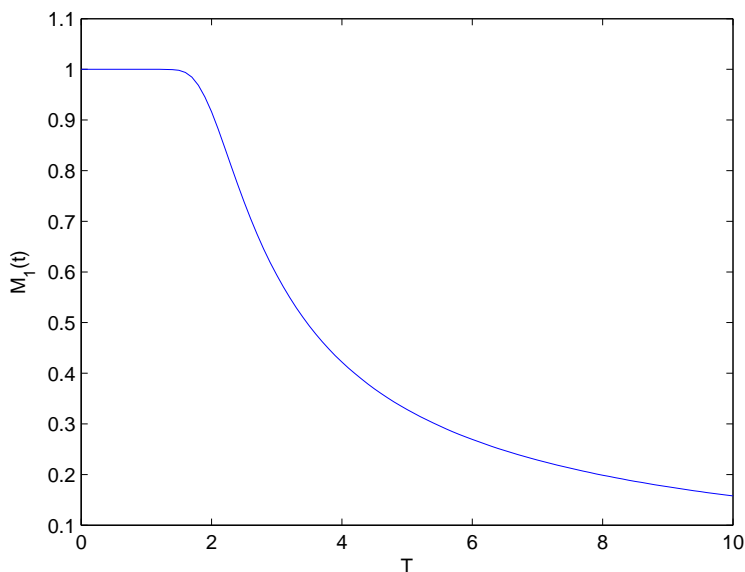


Figure 2.6: $M_1(t)$ for (2.3.7) with $a_{jk} = (jk)^{3/4}$, $b_{jk} = 0$ and $n = 100$.

Example A2 Let $\alpha = 3/4$ so that $a_{jk} = (jk)^{3/4}$. Figure 2.6 shows a sharp decay in $M_1(t)$ at approximately $t = 2$. Numerical results show that this decay continues for larger times. This indicates that there is gelation.

Examples B

Let $a_{jk} = jk$, $b_{jk} = b$. The case $b = 0$ was considered in the previous example. Recall that $M_1(0) = 1$. The calculation in Section 2.2 show that we have gelation if $b < 1$, while if $b > 6$ there is no gelation. These are estimates and we study numerically the examples $b = 2$ and $b = 5$.

For the number of equations n in (2.3.7) we consider both $n = 10$ and $n = 100$. The reason for this is that gelation in the infinite model is the result of large clusters. As we increase n , the fragmentation may delay the formation of these large clusters. Our numerical results will demonstrate this.

Example B1 For this example $a_{jk} = jk$ and $b_{jk} = 2$. Figure 2.7 shows the numerics for $n = 10$ and $t \leq 10$. Note that the decrease in $M_1(t)$ appears to happen before $t = 1$ in Example A1. This is because $n = 100$ for Example A1. Figure 2.8 shows the numerics for $n = 10$ and $t \leq 10^4$. The density $M_1(t)$ continues to decay but at a rate slower than in Example A1.

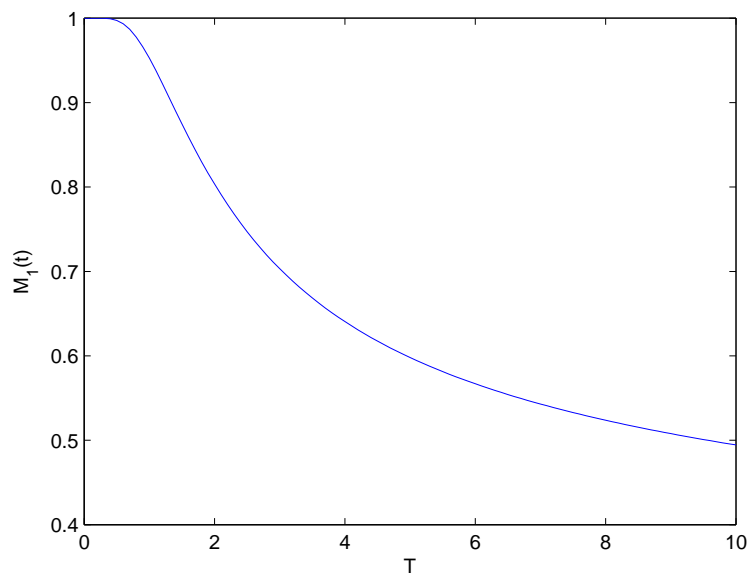


Figure 2.7: $M_1(t)$ for (2.3.7) with $a_{jk} = jk$, $b_{jk} = 2$ and $n = 10$.

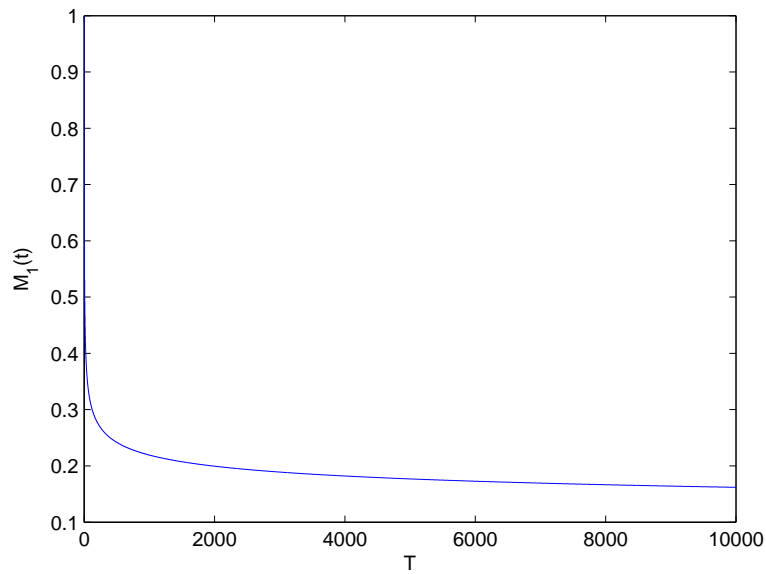


Figure 2.8: $M_1(t)$ for (2.3.7) with $a_{jk} = jk$, $b_{jk} = 2$ and $n = 10$.

Figure 2.9 shows $M_1(t)$ for $n = 100$ and $t \leq 10$. The sharp decrease in $M_1(t)$ now appears to begin near $t = 3$. Also, $M_1(t)$ decays much slower for $n = 100$ compared with the $n = 10$ case. Figure 2.10 shows that again for $n = 100$, $M_1(t)$ decays slower than the $n = 10$ case.

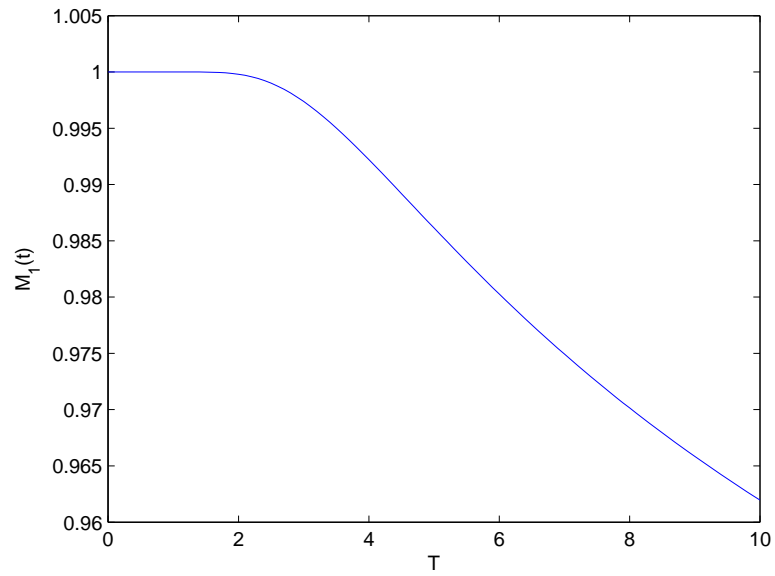


Figure 2.9: $M_1(t)$ for (2.3.7) with $a_{jk} = jk$, $b_{jk} = 2$ and $n = 100$.

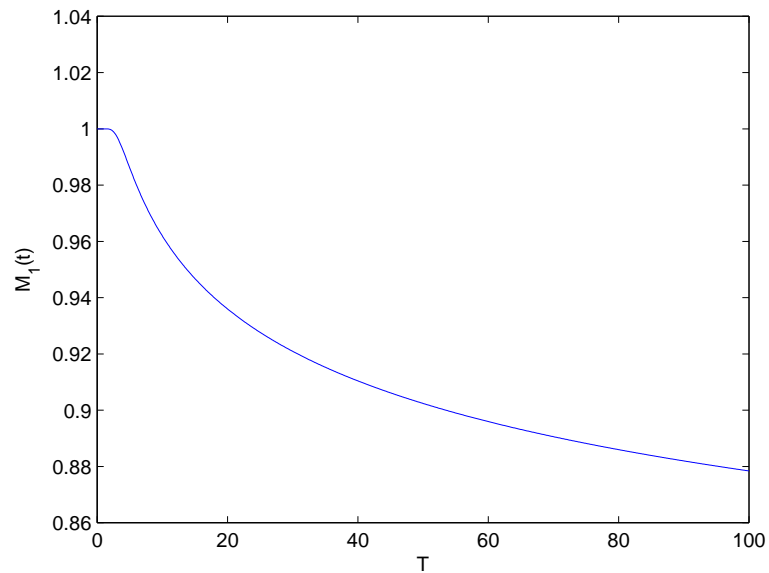


Figure 2.10: $M_1(t)$ for (2.3.7) with $a_{jk} = jk$, $b_{jk} = 2$ and $n = 100$.

Example B2 Let $a_{jk} = jk$, $b_{jk} = 5$. Figure 2.11 and 2.12 show the numerics for $n = 10$. In Figure 2.11, the decrease in $M_1(t)$ appears to begin before $t = 1$ and Figure 2.12 shows that this decay continues for $t \leq 10^4$. This indicates gelation. However Figure 2.13 shows that when $n = 100$ $M_1(t)$ is approximately constant for $t \leq 10^2$. This shows that more tests are needed to verify gelation.

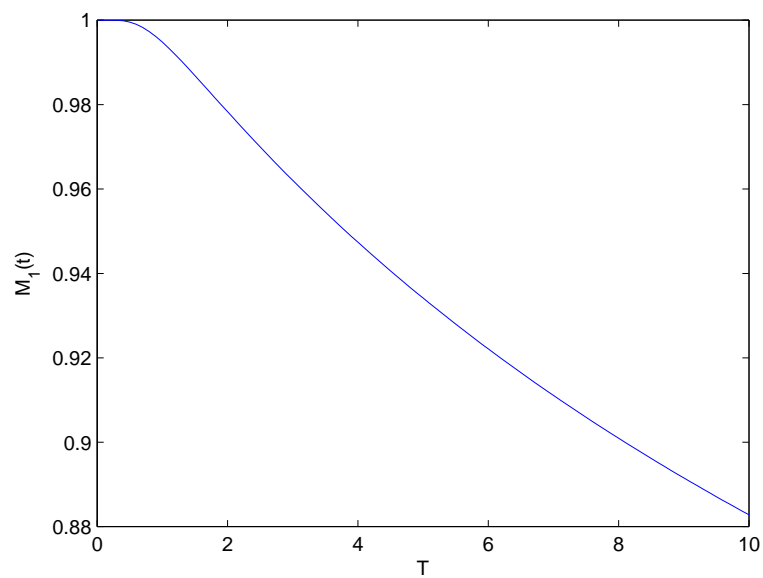


Figure 2.11: $M_1(t)$ for (2.3.7) with $a_{jk} = jk$, $b_{jk} = 5$ and $n = 10$.

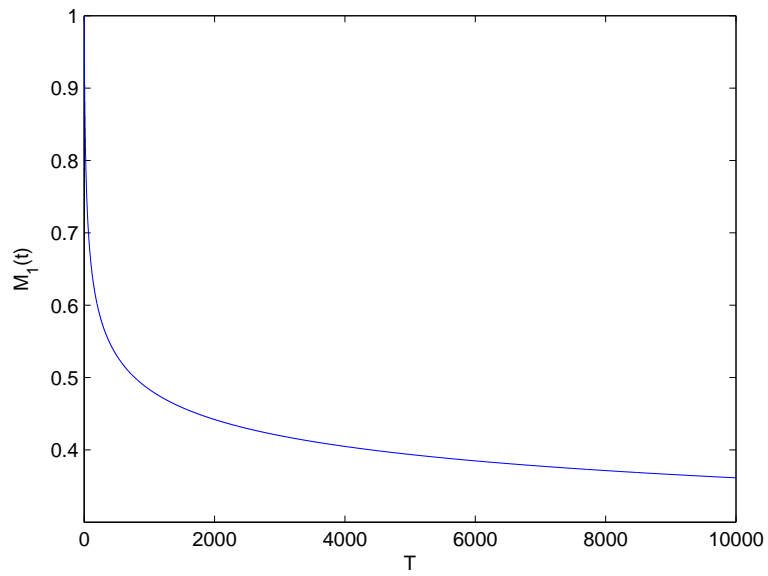


Figure 2.12: $M_1(t)$ for (2.3.7) with $a_{jk} = jk$, $b_{jk} = 5$ and $n = 10$.

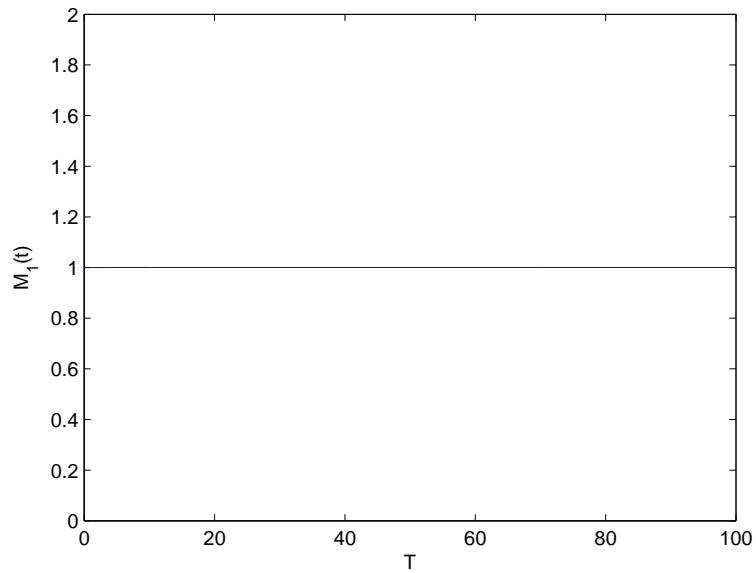


Figure 2.13: $M_1(t)$ for (2.3.7) with $a_{jk} = jk$, $b_{jk} = 5$ and $n = 100$.

Examples C

For this set of examples, we consider the coefficients studied in Example 2 of Section 2.2:

$$a_{jk} = jk, \quad b_{jk} = \frac{b(j+k)^{\alpha+1}}{(jk)^\alpha}. \quad (2.4.2)$$

If $\alpha > 1$ and $b \geq 0$ is small then we expect gelation. If $\alpha \leq 1$ and b is large enough then $M_1(t)$ will be conserved.

Example C1 Let $\alpha = 3$, $b = 1$, $n = 100$ and $t \leq 10^4$. Figure 2.14 indicates that there is no gelation for this case. Increasing the time to 10^5 shows again that $M_1(t)$ is conserved.

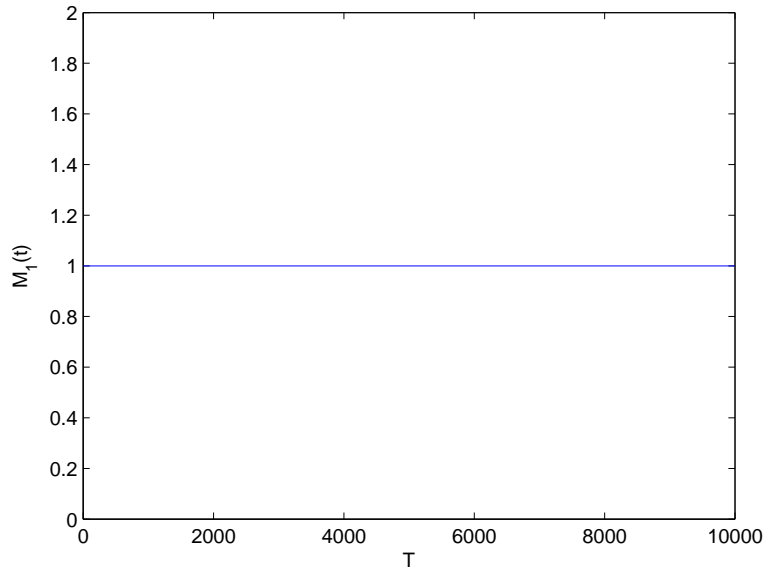


Figure 2.14: $M_1(t)$ for (2.3.7) with $\alpha = 3$, $b = 1$ in (2.4.2) and $n = 100$.

Example C2 For this case we take $\alpha = 3$ and $n = 100$ as in the previous example but we decrease b to $b = 0.5$. Figure 2.15 shows that $M_1(t)$ decreases rapidly

near $t = 1$.

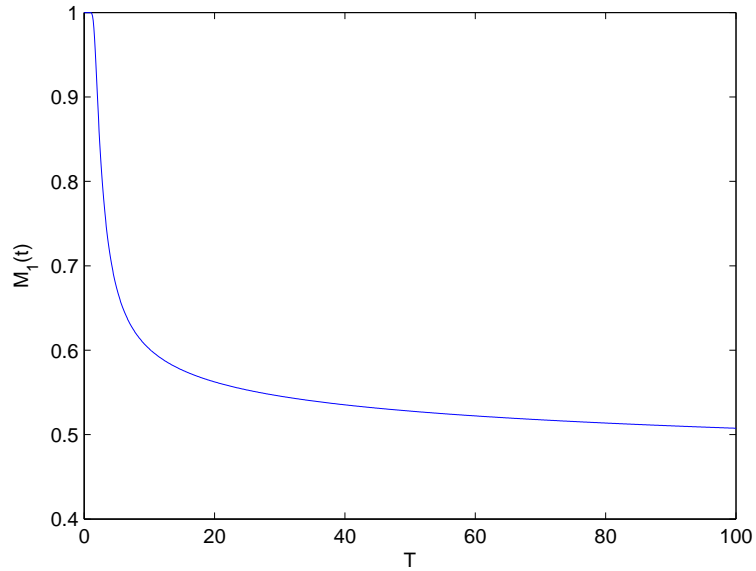


Figure 2.15: $M_1(t)$ for (2.3.7) with $a_{jk} = jk$, $b_{jk} = \frac{b(j+k)^{\alpha+1}}{(jk)^\alpha}$ when $\alpha = 3$, $b = 0.5$ and $n = 100$.

Example C3 Let $\alpha = 1$, $b = 0.6$ and $n = 100$. Figure 2.16 shows that $M_1(t)$ remains constant for $t \leq 10^2$.

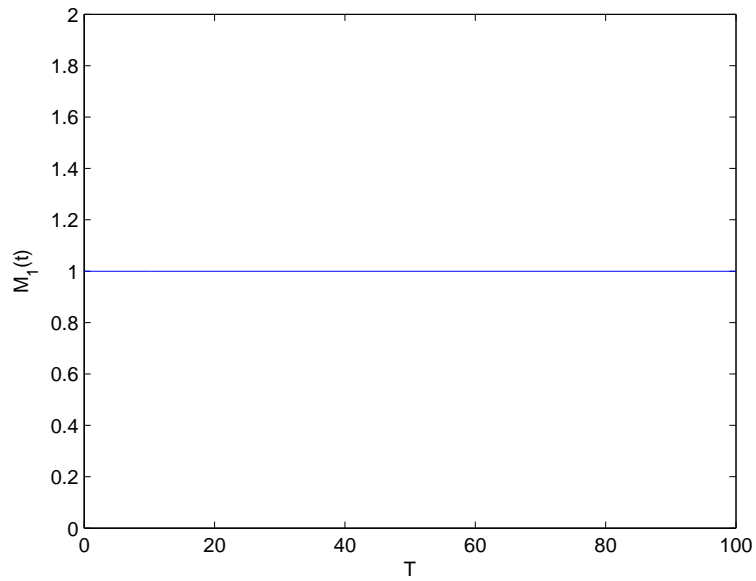


Figure 2.16: $M_1(t)$ for (2.3.7) with $a_{jk} = jk$, $b_{jk} = \frac{b(j+k)^{\alpha+1}}{(jk)^\alpha}$ when $\alpha = 1$, $b = 0.6$ and $n = 100$.

Example C4 We let $\alpha = 1$ and $n = 100$ as in Example C3 but decrease b to $b = 0.2$. Figure 2.17 shows a rapid decrease in $M_1(t)$ near $t = 1$. Figure 2.18 shows that $M_2(t)$ increases rapidly near the same value of t .

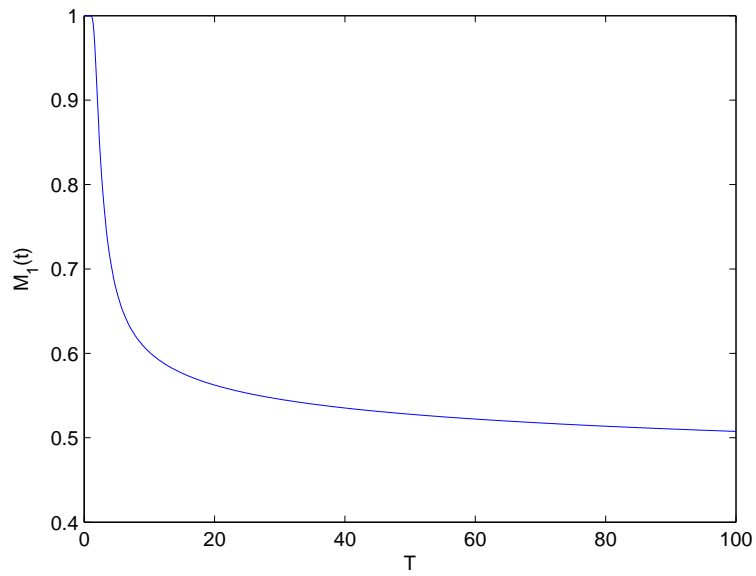


Figure 2.17: $M_1(t)$ for (2.3.7) with $a_{jk} = jk$, $b_{jk} = \frac{b(j+k)^{\alpha+1}}{(jk)^\alpha}$ when $\alpha = 1$, $b = 0.2$ and $n = 100$.

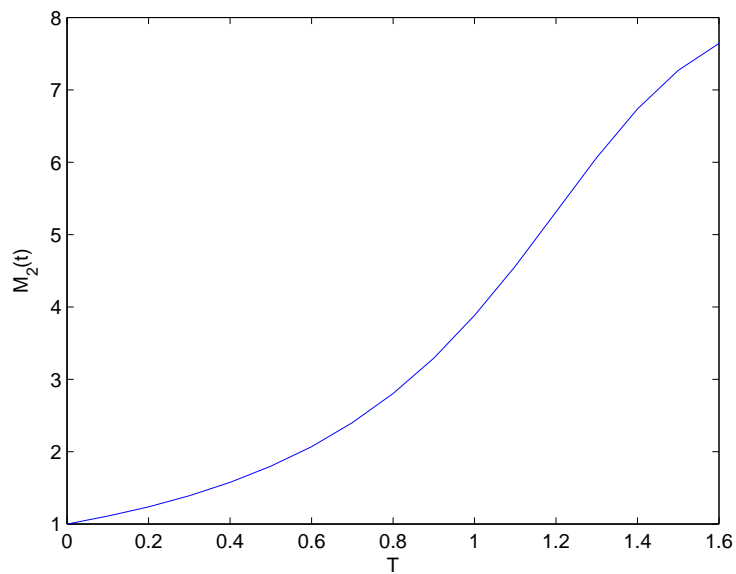


Figure 2.18: $M_2(t)$ for $a_{jk} = jk$, $b_{jk} = \frac{b(j+k)^{\alpha+1}}{(jk)^\alpha}$ when $\alpha = 1$, $b = 0.2$ and $n = 100$.

Chapter 3

Asymptotics for the finite dimensional case

3.1 Introduction

In this chapter we study the large time behaviour of

$$c_j' = \frac{1}{2} \sum_{k=1}^{j-1} W_{j-k,k} - \sum_{k=1}^{n-j} W_{jk} - \sum_{k=n-j+1}^n a_{j,k} c_j c_k, \quad (3.1.1)$$

where

$$W_{j,k} = a_{j,k} c_j c_k - b_{j,k} c_{j+k}.$$

In general solutions of (3.1.1) converge to zero. We study the rate of this convergence.

In Sections 3.2 - 3.4 we study (3.1.1) when both coagulation and fragmentation are included. Numerical studies indicate that the convergence is very slow for this case. We prove this for the detailed balance case giving a general result.

In Section 3.5 - 3.8 we only consider the coagulation case. It turns out that this

is more complicated than the detailed balance case.

3.2 Coagulation-fragmentation dynamics

We consider the coagulation - fragmentation equation under the assumption that we have detailed balance, that is there exists sequence (Q_j) with $Q_1 = 1$ and

$$a_{j,k}Q_jQ_k = b_{j,k}Q_{j+k},$$

for all j and k where $Q_j > 0$ for all j . For either the infinite set of equations or the maximal n -truncation (2.3.1), the equilibrium solutions are given by

$$c_r = Q_r z^r,$$

where $z \geq 0$ is a parameter. For the finite dimensional system (3.1.1) and

$$\rho(t) = \sum_{r=1}^n r c_r(t) \tag{3.2.1}$$

we have that

$$\rho'(t) = - \sum_{j=1}^n j \sum_{k=n-j+1}^n a_{j,k} c_j c_k. \tag{3.2.2}$$

Using (3.2.2) and assuming that $a_{1,n} > 0$ and $b_{1,n} > 0$ for all n we can show that $\rho(t)$ converges to zero at $t \rightarrow \infty$. We will study the rate of this decay.

The aim of the next two sections is to show that for small $c_r(t)$ we have that

$$c_r(t) = Q_r (u(t))^r.$$

where $u(t)$ decays very slowly to zero. This provides some explanation as to why in numerical calculations we see that solutions behave like equilibria at least for moderately large times.

In fact we show that $u(t)$ satisfies an equation of the form

$$\frac{du}{dt} = -ku^{n+1}(1 + O(u)). \quad (3.2.3)$$

for u small. Here k is a constant which depends on the coefficients. The solution of the above equation is

$$u(t) \approx At^{-\frac{1}{n}}.$$

with $A > 0$ a function of k and n , which shows the very slow decay of $u(t)$. We first study the Becker-Döring equations. The results for the general case include this special case. However, the methods introduced for the Becker-Döring case indicate the techniques needed for the general case and for this reason we study it first.

3.3 Becker-Döring equation

In Section 1.2 we introduce the Becker-Döring equations with $a_{j,k} = b_{j,k} = 0$ if both j and k are greater than 1. For the Becker-Döring equations we take that $a_{n,1} = a_n$,

$b_{n,1} = b_n$ and the finite dimensional system (3.1.1) reduces to

$$\begin{aligned} c_1' &= -J_1 - \sum_{j=1}^{n-1} J_r - a_n c_1 c_n \\ c_r' &= J_{r-1} - J_r \\ c_n' &= J_{n-1} - a_n c_1 c_n \end{aligned} \tag{3.3.1}$$

where

$$J_r = a_r c_r c_1 - b_{r+1} c_{r+1}.$$

We will assume that all of the constants a_r and b_r are positive.

For the density $\rho(t)$ given by (3.2.1) we have that

$$\rho'(t) = -a_n(n+1)c_1c_n, \tag{3.3.2}$$

so that $\rho(t)$ is decreasing. We show that the only equilibrium solution of (3.3.1) is the zero solution so that $\rho(t)$ converges to zero.

Lemma 3.3.1. *The only equilibrium solution to (3.3.1) is $c = 0$.*

Proof: Let c be an equilibrium solution. From (3.3.2) we have that

$$c_1 c_n = 0. \tag{3.3.3}$$

We first assume that

$$c_n = 0 \quad , \quad c_1 > 0. \tag{3.3.4}$$

Since $c'_n = 0$ we have that $J_{n-1} = 0$ so that

$$a_{n-1}c_1c_{n-1} - b_n c_n = 0.$$

From (3.3.4) it follows that

$$c_{n-1} = 0. \tag{3.3.5}$$

From $c'_{n-1} = 0$ we have that $J_{n-2} = J_{n-1} = 0$ so that

$$a_{n-2}c_1c_{n-2} - b_{n-1}c_{n-1} = 0.$$

From (3.3.4) and (3.3.5), this shows that

$$c_{n-2} = 0.$$

Proceeding in this way we obtain $c_r = 0$ for $2 \leq r \leq n$. From $c'_2 = 0$ we have $J_1 = 0$ so that $c_1 = 0$ which shows (3.3.4) does not hold.

It follows from (3.3.3) that $c_1 = 0$. Again, since $c'_n = 0$ we have $c_1 = c_n = 0$.

From the fact that $c'_{n-1} = 0$ we obtain $c_{n-1} = 0$. Following this procedure we obtain

$$c_r = 0 \quad , \quad 2 \leq r \leq n$$

and this together with $c_1 = 0$ proves the result.

We use centre manifold theory to study small solutions of (3.3.1). We first need

to change variables so that the linear part is in the correct form, that is,

$$x' = 0 \quad , \quad y' = By$$

with $x \in \mathbb{R}, y \in \mathbb{R}^{n-1}$ and the eigenvalues of B all have negative real parts. To do this we change from (c_1, c_2, \dots, c_n) to x, y where

$$y_r = c_r \quad , \quad 2 \leq r \leq n \tag{3.3.6}$$

$$x = \sum_{r=1}^n r c_r.$$

Since

$$x' = -(n+1)a_n c_1 c_n$$

we have that

$$x' = -(n+1)a_n c_n \left(x - \sum_{r=2}^n r y_r \right) = f(x, y) \tag{3.3.7}$$

which is of the correct form.

To write down the other $n-1$ equations we first note that for $3 \leq r \leq n-1$

$$y'_r = -b_r y_r + b_{r+1} y_{r+1} + c_1 (a_{r-1} y_{r-1} - a_r y_r)$$

while

$$y'_2 = -b_2 y_2 + b_3 y_3 + c_1 (a_1 c_1 - a_2 y_2)$$

and

$$y'_n = -b_n y_n + a_{n-1} c_1 y_{n-1} - a_n c_1 y_n$$

with

$$c_1 = x - \sum_{r=2}^n r y_r.$$

The linear part of the y equation is given by $y' = By$ where we label the elements of B as $(B)_{j,k}$ for $2 \leq j, k \leq n$. From the above calculations

$$(B)_{r,r} = -b_r \quad , \quad 2 \leq r \leq n$$

$$(B)_{r,r+1} = b_{r+1} \quad , \quad 2 \leq r \leq n-1$$

and all other entries of B are zero. It follows that the eigenvalues of B are $-b_2, -b_3, \dots, -b_n$ and that they are all negative.

To write the nonlinear part of the y equations we define $g : \mathbb{R}^n \rightarrow \mathbb{R}^{n-1}$ with components g_2, g_3, \dots, g_n where for $3 \leq r \leq n$,

$$g_r(x, y) = (a_{r-1}y_{r-1} - a_r y_r) \left(x - \sum_{r=2}^n r y_r \right),$$

$$g_2(x, y) = (a_1 x - a_1 \sum_{r=2}^n r y_r - a_2 y_2) \left(x - \sum_{r=2}^n r y_r \right).$$

Hence the equations are

$$\begin{aligned} x' &= f(x, y) \\ y' &= By + g(x, y) \end{aligned} \tag{3.3.8}$$

where $f(x, y)$ is defined in (3.3.7).

It follows from the general theory described in Section 1.5 that there is a centre manifold for (3.3.8) given by $y = h(x)$ with $h : \mathbb{R} \rightarrow \mathbb{R}^{n-1}$ and $h(x) = O(x^2)$ as $x \rightarrow 0$. The dynamics on the centre manifold is given by the scalar equation

$$u' = f(u, h(u)). \quad (3.3.9)$$

This equation captures the local dynamics of the full system except for an exponentially small term of order e^{-pt} with $p > 0$.

In order to study solutions to (3.3.9) we need to find an approximation to the centre manifold $h(u)$. We use the general theory described in Section 1.5 to do this.

Let $\phi : \mathbb{R} \rightarrow \mathbb{R}^{n-1}$ with $\phi(0) = 0$, $\phi'(0) = 0$, so that $\phi(u) = O(u^2)$.

Let

$$(M\phi)(u) = \phi'(u)f(u, \phi(u)) - B\phi(u) - g(u, \phi(u)). \quad (3.3.10)$$

The centre manifold satisfies $(Mh)(u) \equiv 0$. The theory tells us that if we can find $\phi(u)$ such that

$$(M\phi)(u) = O(|u|^q)$$

for some $q \geq 2$ then

$$h(u) = \phi(u) + O(|u|^q).$$

We expect that the $\phi'(u)f(u, \phi(u))$ term in (3.3.10) to be of higher order than the other terms. Hence to get a good approximation to $M\phi$ we need to choose ϕ so that

$$B\phi(u) + g(u, \phi(u))$$

is small. The above expression is the right hand side of the Becker-Döring equations (3.3.1). For $3 \leq r \leq n - 1$ the r component of this is

$$J_{r-1} - J_r.$$

So the idea is to make $J_r \equiv 0$, that is, ϕ_r should be an equilibrium with $J_r = 0$ so that

$$\phi_r = Q_r z^r \tag{3.3.11}$$

with z to be determined. For the Becker-Döring equations the sequence Q_r is given by $Q_1 = 1$ and for $r \geq 1$,

$$a_r Q_r = b_{r+1} Q_{r+1}. \tag{3.3.12}$$

For $r \geq 2$ we have that

$$J_r = a_r \phi_r \left(u - \sum_{r=2}^n r \phi_r \right) - b_{r+1} \phi_{r+1}$$

with ϕ_r given by (3.3.11). We can write this as

$$J_r = a_r Q_r z^r \left(u - \sum_{r=2}^n r Q_r z^r \right) - b_{r+1} Q_{r+1} z^{r+1}.$$

For $r \geq 2$, using (3.3.12)

$$J_r = a_r Q_r z^r \left(u - \sum_{r=1}^n r Q_r z^r \right). \tag{3.3.13}$$

To make $J_r = 0$ we need

$$u - \sum_{r=1}^n rQ_r z^r = 0.$$

This informs us how to define z .

Since the function

$$\sum_{r=1}^n rQ_r z^r$$

is a strictly increasing function of z , for each $u > 0$ there is a unique $z = z(u)$ such that

$$u = \sum_{r=1}^n rQ_r (z(u))^r. \quad (3.3.14)$$

With this definition of z we see from (3.3.13) that $J_r = 0$ for $r \geq 2$. Also

$$\begin{aligned} J_1 &= a_1 \left(u - \sum_{r=2}^n rQ_r z^r \right)^2 - b_2 Q_2 z^2 \\ &= a_1 z^2 - b_2 Q_2 z^2 \\ &= 0 \end{aligned}$$

since $a_1 Q_1 = b_2 Q_2$ and $Q_1 = 1$. Hence we have that $J_r = 0$ for all r .

We also note from the definition of z that

$$z(u) = u + O(u^2). \quad (3.3.15)$$

We now show that

$$(M\phi)(u) = O(|u|^{n+1}). \quad (3.3.16)$$

We begin the proof of this by estimating the r component of $\phi'(u)f(u, \phi(u))$ which is given by

$$-rQ_r z^{r-1}(n+1)a_n Q_n z^n \left(u - \sum_{r=2}^n rQ_r z^r\right).$$

From the definition of $z(u)$ this is equal to

$$-rQ_r Q_n (n+1)z^{n+r}.$$

Since $r \leq 2 \leq n$ this term is $O(z^{n+2})$ and using (3.3.15) it is $O(u^{n+2})$.

Next we estimate the r component of $B\phi + g(u, \phi(u))$. For $2 \leq r \leq n-1$ this is equal to $J_{r-1} - J_r$ and this is zero since $J_r = 0$. The n component is given by

$$J_{n-1} - \left(u - \sum_{r=2}^n rQ_r z^r\right)a_n Q_n z^n.$$

We have $J_{n-1} = 0$ and from the definition of $z(u)$ the other term is $O(z^{n+1}) = O(u^{n+1})$.

This completes the proof of (3.3.16).

It follows that

$$h(u) = \phi(u) + O(u^{n+1}),$$

so that for $r \leq 2 \leq n$

$$h_r(u) = Q_r(z(u))^r + O(u^{n+1}). \quad (3.3.17)$$

The equation on the centre manifold is

$$u' = f(u, h(u))$$

and

$$f(u, h(u)) = -(n+1)a_n h_n(u) \left(u - \sum_{r=2}^n r h_r(u) \right).$$

From (3.3.17)

$$h_n(u) = Q_n z^n + O(u^{n+1}) = Q_n u^n + O(u^{n+1}).$$

Also,

$$\begin{aligned} u - \sum_{r=2}^n r h_r(u) &= u - \sum_{r=2}^n r Q_r z^r + O(u^{n+1}) \\ &= z + O(u^{n+1}) \\ &= u + O(u^{n+1}). \end{aligned}$$

It follows that the equation on the centre manifold is

$$u' = -(n+1)a_n Q_n u^{n+1} + O(u^{n+2}). \quad (3.3.18)$$

Lemma 3.3.2. Consider the scalar differential equation $w' = F(w)$

where

$$F(w) = -kw^\alpha(1 + O(w)) \text{ as } w \rightarrow 0$$

with $k > 0$ and $\alpha > 1$. Let $w(0) > 0$ and $p = (\alpha - 1)$.

Then

$$\lim_{t \rightarrow \infty} t^{1/p} w(t) = \frac{1}{(k(\alpha - 1))^{1/p}}.$$

Proof: Clearly $w(t) \rightarrow 0$ as $t \rightarrow \infty$ so we can write the $O(w)$ term as $o(1)$ as $t \rightarrow \infty$. Integrating the differential equation gives

$$w^{-p} = kt(1 + o(1)) + c$$

where c is a positive constant so that

$$w(t) = \frac{1}{(k(\alpha - 1))^{1/p}(t + o(t) + c_1)^{1/p}}$$

where c_1 is another positive constant. The result follows.

As well as the one dimensional centre manifold, the zero solution of equation (3.3.1) has an $(n - 1)$ dimensional stable manifold. On the stable manifold, solutions converges exponentially fast to zero. Taking initial data on the stable manifold means that $u(0) = 0$ for the centre manifold equation. Most initial data for (3.3.1) will not be on the stable manifold so in general we will have $u(0) > 0$.

Applying (3.3.2) to the centre manifold equation (3.3.18) we arrive at our result on asymptotic behaviour.

Theorem 3.3.3. *If the initial data for (3.3.1) is not on the stable manifold then*

$$\lim_{t \rightarrow \infty} t^{1/n} c_1(t) = \frac{1}{((n^2 + n)a_n Q_n)^{1/n}}.$$

We present some numerical results which illustrate Theorem 3.3.3. In all cases we

have that $c_1(0) = 1$ while $c_j(0) = 0$ for $j \geq 2$ so that $M_1(0) = 1$.

Example A Let $a_n = b_{n+1} = 1$ for all n . For this case $Q_n = 1$ for all n .

Figure 3.1 shows $M_1(t)$ for the case $n = 6$. The density $M_1(t)$ is decreasing slowly.

Figure 3.2 shows the graph of

$$t^{1/n}c_1(t)[(n^2 + n)a_nQ_n]^{1/n} \quad (3.3.19)$$

for $n = 6$. The prediction from Theorem 3.3.3 is that this quantity converges to 1.

The numerics support this.

Figure 3.3 shows $M_1(t)$ for the case $n = 10$. Here the density converges slower than the case shown in Figure 3.1. The quantity $M_1(t)$ is shown in Figure 3.4 for the $n = 20$ case. After time 10^6 , the density has decreased by about 2%.

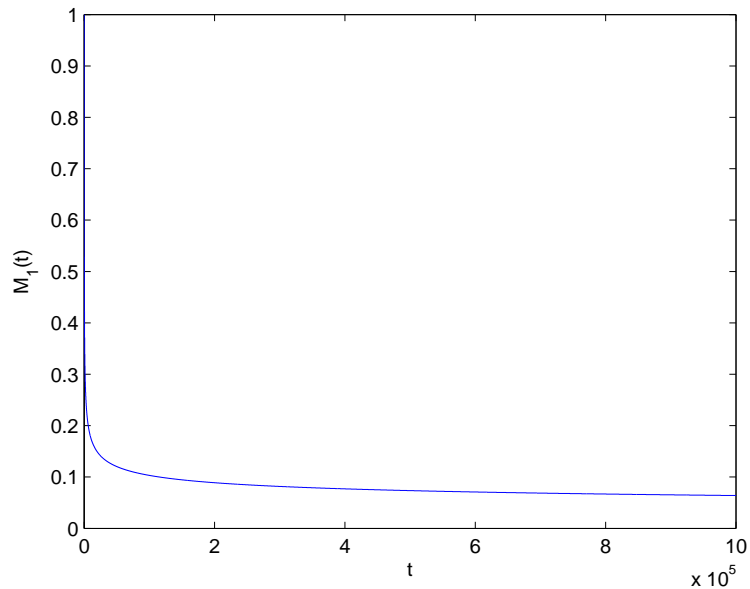


Figure 3.1: Graph of $M_1(t)$ for $n = 6$. See Example A.

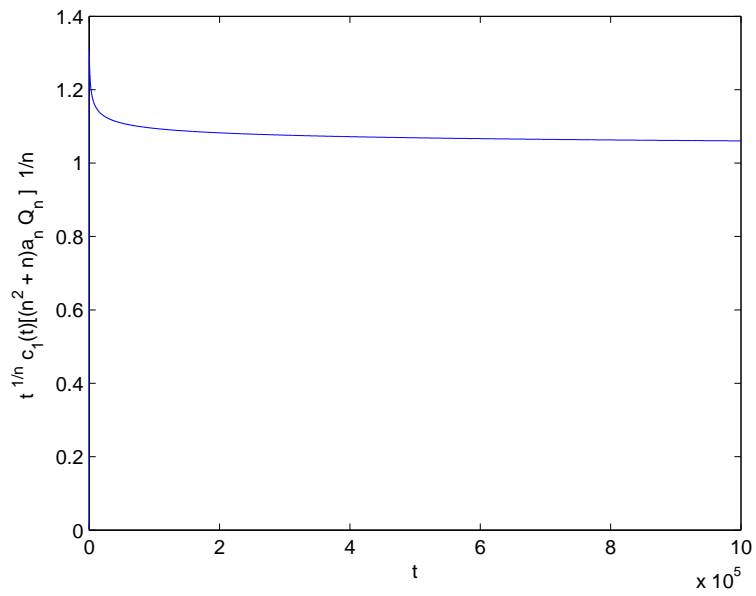


Figure 3.2: Graph of $t^{1/n} c_1(t) [(n^2 + n)a_n Q_n]^{1/n}$ for $n = 6$. See Example A.

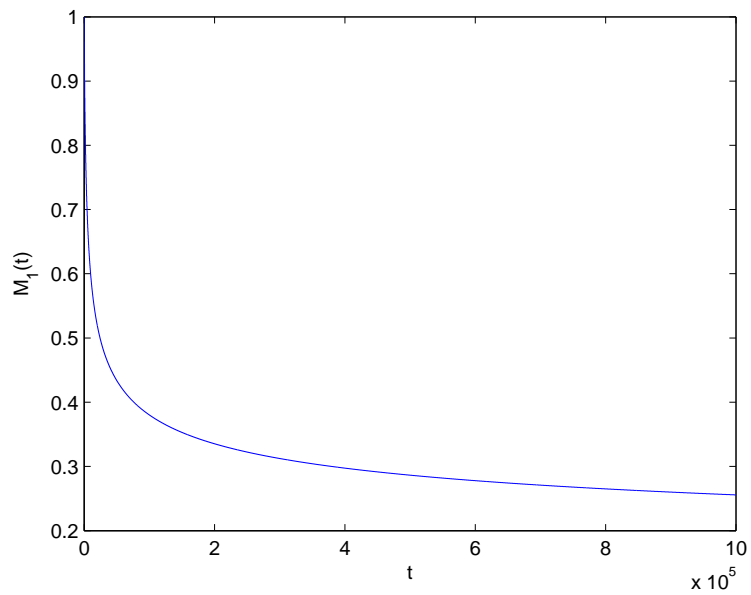


Figure 3.3: Graph of $M_1(t)$ for $n = 10$. See Example A.

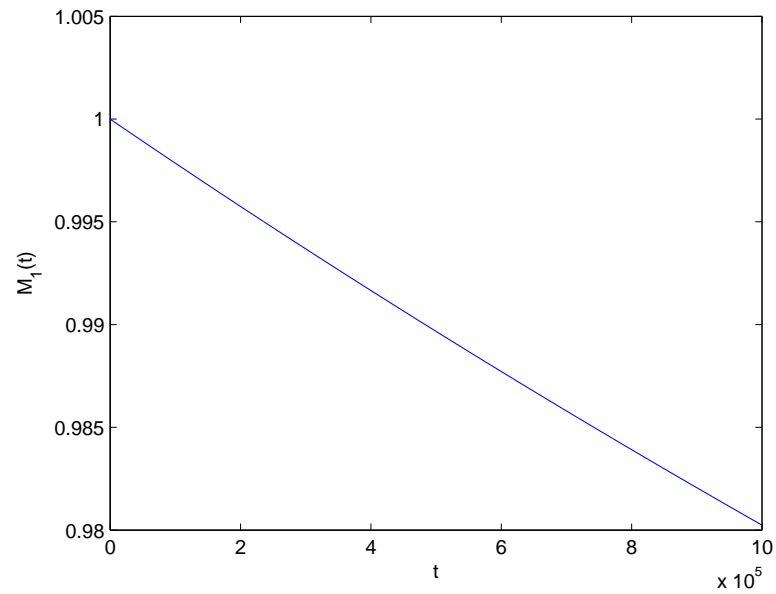


Figure 3.4: Graph of $M_1(t)$ for $n = 20$. See Example A.

Example B Let $a_n = b_{n+1} = \sqrt{n}$ so that $Q_n = 1$ for all n . For these results we take $n = 6$. Figure 3.5 shows $M_1(t)$ while Figure 3.6 shows the quantity (3.3.19). The coefficients a_n and b_{n+1} are bigger than those of Example A and for this reason the solutions appear to converge quicker.

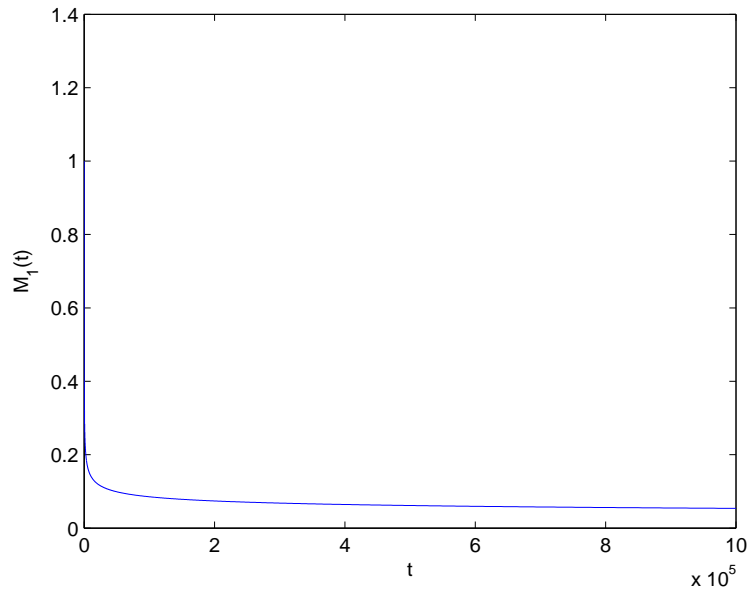


Figure 3.5: Graph of $M_1(t)$. See Example B.

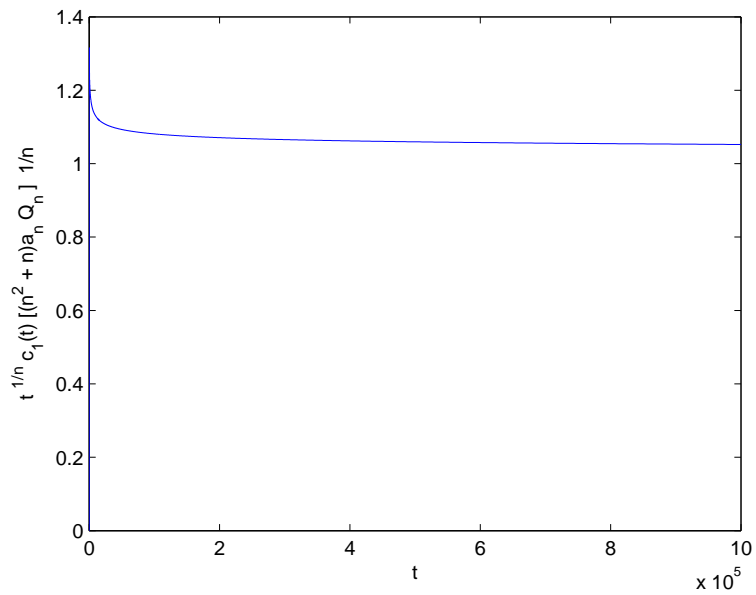


Figure 3.6: Graph of $t^{1/n} c_1(t) [(n^2 + n)a_n Q_n]^{1/n}$. See Example B.

3.4 The general case with detailed balance

For the general case, the finite dimensional system is

$$c'_j = \frac{1}{2} \sum_{k=1}^{j-1} W_{j-k,k} - \sum_{k=1}^{n-j} W_{j,k} - \sum_{k=n-j+1}^n a_{j,k} c_j c_k, \quad (3.4.1)$$

for $j = 1, 2, \dots, n$ where

$$W_{j,k} = a_{j,k} c_j c_k - b_{j,k} c_{j+k}.$$

As well as the assumption made about detailed balance in Section (3.2), we assume that for all k

$$a_{1,k} > 0 \quad , \quad b_{1,k} > 0. \quad (3.4.2)$$

From Section (3.2), the density $\rho(t)$ is decreasing. We show that zero is the only equilibrium solution to (3.4.1) so that $\rho(t)$ converges to zero.

Lemma 3.4.1. *The only equilibrium solution of (3.4.1) is $c = 0$.*

Proof: This will be very similar to the corresponding result Lemma 3.3.1 for the Becker-Doring equations. We only give a brief outline of the proof.

Let c be an equilibrium solution. From (3.2.2) for all j ,

$$\sum_{k=n-j+1}^n a_{j,k} c_j c_k = 0.$$

Taking $j = 1$ and using $a_{1,n} > 0$ we obtain

$$c_1 c_n = 0.$$

We first assume that

$$c_n = 0 \quad , \quad c_1 > 0. \quad (3.4.3)$$

Since $c'_n = 0$

$$\frac{1}{2} \sum_{k=1}^{n-1} a_{n-k,k} c_{n-k} c_k - c_n \sum_{k=1}^{n-1} b_{n-k,k} = 0.$$

Using (3.4.3) and $a_{n-1,1} > 0$ gives $c_{n-1} = 0$. From $c'_n = 0$ and $c_{n-1} = c_n = 0$ we obtain

$$\sum_{k=1}^{n-2} a_{n-1-k,k} c_{n-1-k} c_k = 0.$$

Since $a_{n-2} > 0$ and $c_1 \neq 0$ we obtain $c_{n-2} = 0$.

Continuing in this way we obtain $c_1 = 0$ so that (3.4.3) can not hold. Hence $c_1 = 0$. Using $c'_k = 0$ starting with $k = n$ as in the proof of Lemma 3.3.1, we obtain $c_k = 0$ for all k as required.

We again apply centre manifold theory to study small solutions of (3.4.1). We begin by making the change of variables

$$y_r = c_r \quad , \quad 2 \leq r \leq n \quad (3.4.4)$$

$$x = \sum_{r=1}^n r c_r.$$

We write $y = [y_2, y_3, \dots, y_n]^T$ so $y \in \mathbb{R}^{n-1}$.

For ease of notation in writing down the equations we make use of y_1 defined by

$$y_1 = x - \sum_{r=2}^n r y_r. \quad (3.4.5)$$

The scalar y_1 is not part of the vector y .

The system of equation (3.4.1) can be written as

$$\begin{aligned}x' &= f(x, y) \\y' &= By + g(x, y).\end{aligned}\tag{3.4.6}$$

From (3.2.2)

$$f(x, y) = - \sum_{j=1}^n j \sum_{k=n-j+1}^n a_{j,k} y_j y_k,\tag{3.4.7}$$

with y_1 given by (3.4.5).

The matrix B is of size $(n - 1) \times (n - 1)$ and we label its elements as $(B)_{j,k}$ for $2 \leq j, k \leq n$. From (3.4.1) the linear part comes from the contribution of the fragmentation term and is given by

$$(B)_{r,r} = -\gamma_r = -\frac{1}{2} \sum_{k=1}^{r-1} b_{r-k,k} \quad 2 \leq r \leq n,$$

$$(B)_{r,r+k} = b_{r,k} \quad , \quad 2 \leq r \leq n - 1 \quad , \quad k = 1, 2, \dots, n - r.$$

Since B is upper diagonal, it has eigenvalues $-\gamma_r$. Also,

$$\gamma_r \geq \frac{1}{2} b_{r-1,1} > 0,$$

so that all the eigenvalues are negative.

For the nonlinear part of the second equation in (3.3.8). we have that

$g : \mathbb{R}^n \rightarrow \mathbb{R}^{n-1}$ with components g_r , $r = 2, 3, \dots, n$. The components are given by

$$g_r(x, y) = \frac{1}{2} \sum_{k=1}^{r-1} a_{r-k,k} y_{r-k} y_k - \sum_{k=n-r+1}^n a_{r,k} y_r y_k, \quad (3.4.8)$$

with $y_1 = y_1(x, y)$ given by (3.4.5).

It follows that there is a centre manifold $y = h(x)$ with $h : \mathbb{R} \rightarrow \mathbb{R}^{n-1}$. The equation on the centre manifold is

$$u' = f(u, h(u)). \quad (3.4.9)$$

From the formula for f given by (3.4.7) we see that $u' < 0$ so that u will decay to zero. We need a better approximation $h(x) = O(x^2)$ in order to find the decay rate.

Let $\phi : \mathbb{R} \rightarrow \mathbb{R}^{n-1}$ with $\phi(u) = O(u^2)$ as $u \rightarrow 0$ and set

$$(M\phi)(u) = \phi'(u)f(u, h(u)) - B\phi(u) - g(u, \phi(u)). \quad (3.4.10)$$

Our aim is to choose ϕ so that $(M\phi)(u) = O(u^q)$ for some $q > 2$ so that $h(u) = \phi(u) + O(u^q)$. We will write the components of ϕ and h as ϕ_r and h_r for $2 \leq r \leq n$.

For each $u > 0$ let $z(u)$ be the solution of

$$u = \sum_{r=1}^n r Q_r(z(u))^r. \quad (3.4.11)$$

We define $\phi(u)$ by

$$\phi_r(u) = Q_r(z(u))^r \quad r \geq 2$$

so that

$$z(u) = u + O(u^2).$$

We show that with this choice of ϕ ,

$$(M\phi)(u) = O(u^{n+1}). \quad (3.4.12)$$

We first estimate $\phi'(u)f(u, \phi(u))$. Now

$$f(u, \phi) = - \sum_{j=1}^n j \sum_{k=n-j+1}^n a_{j,k} \phi_j \phi_k,$$

where we use the notation

$$\begin{aligned} \phi_1 &= u - \sum_{r=2}^n r \phi_r \\ &= u - \sum_{r=2}^n r Q_r(z(u))^r. \end{aligned}$$

Hence

$$\phi_1(u) = z(u) = u + O(u^2).$$

It follows that $f(u, \phi)$ is of order

$$\sum_{j=1}^n \sum_{k=n-j+1}^n z^{j+k} = O(u^{n+1}).$$

Since

$$\phi'(u) = r Q_r z^{r-1},$$

it follows that

$$\phi'(u)f(u, \phi(u)) = O(u^{n+2}).$$

Next we estimate the r component of the second term of g in equation (3.4.8)

which is

$$\sum_{k=n-j+1}^n a_{j,k} \phi_r \phi_k.$$

Using $\phi_1(u) = O(u)$ this term is of order

$$\sum_{k=n-r+1}^n z^{r+k} = O(z^{n+1}).$$

The remaining terms in $B\phi + g(u, \phi(u))$ involve sums of terms $W_{j,k}$ with

$$W_{jk} = a_{jk} Q_j Q_k - b_{jk} Q_{j+k}.$$

We show that all of these terms are zero.

For $j, k \geq 2$

$$\begin{aligned} W_{jk} &= a_{jk} Q_j Q_k z^{j+k} - b_{jk} Q_{j+k} z^{j+k} \\ &= (a_{jk} Q_j Q_k - b_{jk} Q_{j+k}) z^{j+k} \\ &= 0, \end{aligned}$$

by detailed balance. For $k \geq 2$

$$\begin{aligned}
 W_{1k} &= a_{1k}\phi_1 Q_k z^k - b_{1k} Q_{1+k} z^{1+k} \\
 &= a_{1k} Q_k z^k (u - \sum_{r=2}^n r Q_r z^r) - b_{1k} Q_{k+1} z^{k+1} \\
 &= (a_{1k} Q_k - b_{1k} Q_{k+1}) z^{k+1} \\
 &= 0
 \end{aligned}$$

using $Q_1 = 1$ and detailed balance. Finally,

$$W_{11} = a_{11} z^2 - b_{11} Q_2 z^2 = 0,$$

so all terms involving $W_{j,k}$ are zero. This completes the proof of (3.4.12).

It follows that the components of the centre manifold h are given by

$$h_r(u) = Q_r (z(u))^r + O(u^{n+1}), \quad (3.4.13)$$

for $r \geq 2$. We will use the notation

$$h_1 = h_1(u) = u - \sum_{r=2}^n r h_r(u).$$

From (3.4.13)

$$h_1(u) = u - \sum_{r=2}^n r Q_r z^r + O(u^{n+1}),$$

so that

$$h_1(u) = z + O(u^{n+1}). \quad (3.4.14)$$

The equation on the centre manifold is

$$u' = f(u, h(u)).$$

We have that

$$f(u, h(u)) = - \sum_{j=1}^n j \sum_{k=n-j+1}^n a_{jk} h_j h_k.$$

Using (3.4.13) and (3.4.14)

$$f(u, h(u)) = - \sum_{j=1}^n j \sum_{k=n-j+1}^n a_{jk} Q_j Q_k z^{j+k} + O(u^{n+2}).$$

In the above sum, we only need to keep the terms with $j + k = n + 1$ since the others are $O(u^{n+2})$.

$$f(u, h(u)) = -z^{n+1} \sum_{j=1}^n j a_{j, n-j+1} Q_j Q_{n-j+1} + O(u^{n+2}). \quad (3.4.15)$$

We check that this reduces to (3.3.18) for the Becker-Doring equations. For those equations. $a_{j1} = a_j$ for $j \geq 2$ and $a_{jk} = 0$ for $j, k \geq 2$. Using $Q_1 = 1$,

$$\begin{aligned} \sum_{j=1}^n j a(j, n-j+1) Q_j Q_{n-j+1} &= a(1, n) Q_n + n a(n, 1) Q_n \\ &= (n+1) a_n Q_n \end{aligned}$$

as required.

Applying Lemma 3.3.2 to (3.4.15) gives the decay rate for solutions to (3.4.1).

Theorem 3.4.2. *If the initial data for (3.4.1) is not on the stable manifold then*

$$\lim_{t \rightarrow \infty} t^{1/n} c_1(t) = \left(n \sum_{j=1}^n j a(j, n-j+1) Q_j Q_{n-j+1} \right)^{-\frac{1}{n}}.$$

We now give some numerical results which support the above results.

Example C We let

$$a_{jk} = b_{jk} = 1 \quad \text{for all } j, k,$$

so that $Q_j = 1$ for all j . The initial data is $c_1(0) = 1$ and $c_j(0) = 0$ for $j \geq 2$ so that $M_1(0) = 1$.

For the case $n = 2$, Figure 3.7 shows $M_1(t)$ while Figure 3.8 shows

$$(nA)^{\frac{1}{n}} t^{1/n} c_1(t) = (2A)^{\frac{1}{2}} t^{\frac{1}{2}} c_1(t), \quad (3.4.16)$$

where

$$A = \sum_{j=1}^n j a(j, n-j+1) Q_j Q_{n-j+1} = \frac{n(n+1)}{2}. \quad (3.4.17)$$

The numerics show that $M_1(t)$ converges quickly to 0 while the expression in (3.4.17) converges quickly to 1.

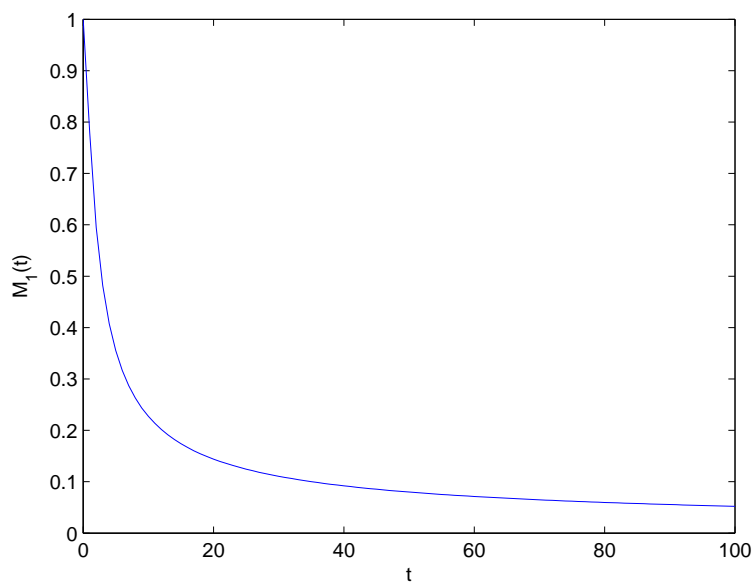


Figure 3.7: Graph of $M_1(t)$ for $n = 2$. See Example C.

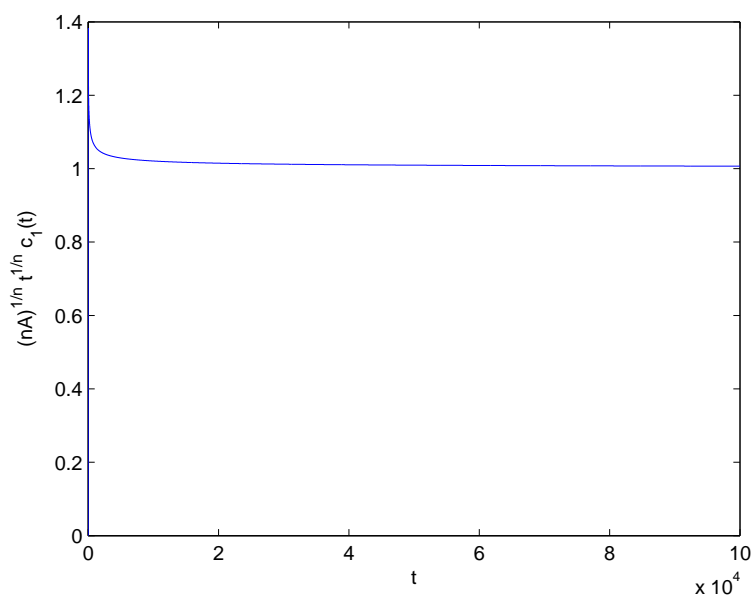


Figure 3.8: Graph of $(nA)^{\frac{1}{n}} t^{1/n} c_1(t)$ for $n = 2$. See Example C.

Figure 3.9 and 3.10 show the same expressions for the case $n = 6$. Even with this modest increase in n , the convergence is much slower.

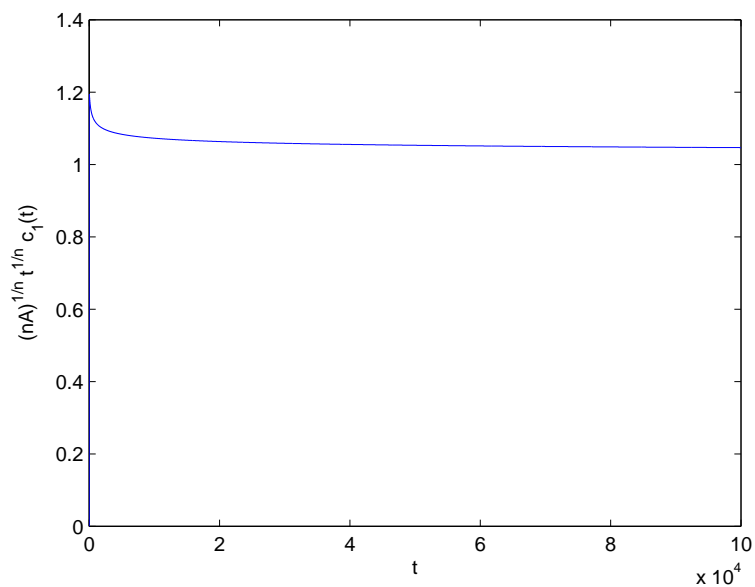


Figure 3.9: Graph of $(nA)^{\frac{1}{n}} t^{1/n} c_1(t)$ for $n = 6$. See Example C.

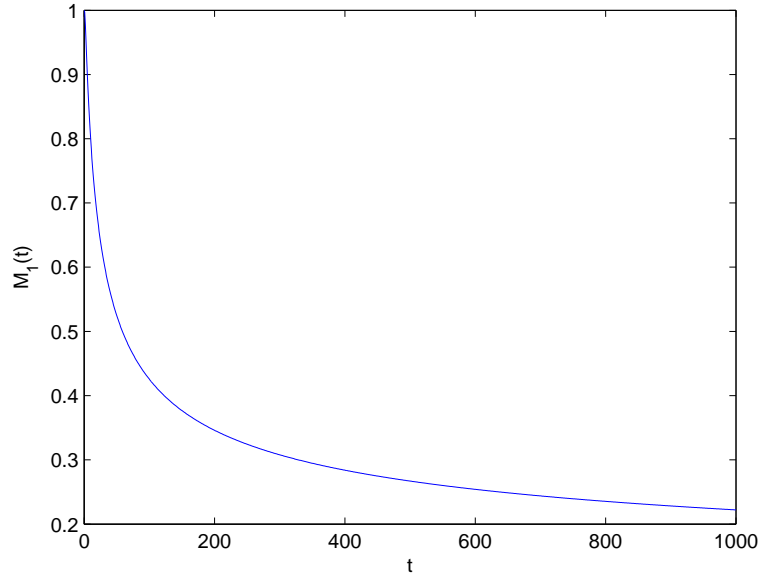


Figure 3.10: Graph of $M_1(t)$ for $n = 6$. See Example C.

3.5 Coagulation dynamics

The minimal n -truncation for the coagulation equation is for $j = 1, 2, \dots, n$

$$c'_j = \frac{1}{2} \sum_{k=1}^{j-1} a_{j-k,k} c_{j-k} c_k - c_j \sum_{k=1}^n a_{j,k} c_k. \quad (3.5.1)$$

We will assume that $a_{1k} > 0$ for all k throughout this section. From (3.2.2) the density is decreasing. In a similar way to Lemma 3.4.1 we can prove that zero is the only equilibrium solution to (3.5.1).

It follows that the density converges to zero. We study the decay rate of solutions. For the general coagulation-fragmentation equation we were able to present a general decay rate. For (3.5.1) the behaviour of solutions for large t is more complicated as

we show in the rest of this chapter.

There have been a number of studies of decay rates for the infinite coagulation equations where the second sum in (3.5.1) has $n = \infty$. However there are very few definite results and some of the claims made are false. Consider the coagulation coefficients

$$a_{j,k} = j^\alpha + k^\alpha \quad (\text{sum kernel}), \quad (3.5.2)$$

and

$$a_{j,k} = (jk)^\alpha \quad (\text{product kernel}). \quad (3.5.3)$$

For the infinite system, it has been claimed [30] that $c_1(t) \sim t^{-1}$ for (3.5.3) and $c_1(t) \sim t^{-\beta}$ for (3.5.2) where $\beta = (2 - \alpha)(2 - 2\alpha)^{-1}$, $\alpha < 1$. For both kernels the claim is that $c_1(t) \sim t^{-1}$ for $\alpha = 0$. This is wrong as $c_1(t) \sim t^{-2}$ for $\alpha = 0$ as can be seen from the exact solution (1.3.7) in Chapter 1.

For (3.5.1) the most significant work is in [11] which considers the product kernel $a_{j,k} = r_j r_k$. This work was motivated by some exact solutions of the infinite system which did not conserve density. Under certain conditions on the sequence (r_j) it was proved that (3.5.1) had solutions of the form

$$c_j(t) = \gamma_j t^{-1}, \quad j = 1, 2, \dots, N, \quad (3.5.4)$$

for some sequence γ_j . It was conjectured in [11] that all solutions to (3.5.1) become close to the solution in (3.5.4) for large t . If this were true it would help in our understanding of the infinite case. So far there has not been any progress on this conjecture.

For the case $a_{j,k} = 1$ there is an exact representation of solutions to (3.5.1) as we will show in the next section. In [31] this was used to predict that for large t

$$c_1(t) \sim \frac{1}{n t (\ln t)}. \quad (3.5.5)$$

In the next section we will prove that

$$\lim_{t \rightarrow \infty} t (\ln t)^{\frac{n-1}{n}} c_1(t) = \left(\frac{2}{n}\right)^{1-\frac{1}{n}}. \quad (3.5.6)$$

We will also determine the large time behaviour of $c_j(t)$ for all j .

In Section 3.7 we will use the idea in [11] to study the possible $O(t^{-1})$ behaviour of solutions to (3.5.1). In the final section we study (3.5.1) for $n = 2$. Even though there are only three parameters in this problem we demonstrate that there is a range of possible decay rates.

3.6 Constant coagulation rates

For $a_{jk} = 1$ for all j and k the coagulation equation becomes

$$c_j' = \frac{1}{2} \sum_{k=1}^{j-1} c_{j-k} c_k - c_j \sum_{k=1}^n c_k. \quad (3.6.1)$$

An exact representation of the solution was given in [31] for the case of monodisperse initial data

$$c_j(0) = 1, c_j(0) = 0, \quad j \geq 2. \quad (3.6.2)$$

Lemma 3.6.1. *The solution of (3.6.1) for initial data (3.6.2) is*

$$c_j(t) = (z(t))^{j-1} e^{-f(z(t))}. \quad (3.6.3)$$

$$f(z) = 2 \sum_{k=1}^n \frac{z^k}{k}. \quad (3.6.4)$$

$$t = 2 \int_0^z e^{f(w)} dw = I(z). \quad (3.6.5)$$

Proof: Because of some errors in [31] we give a complete proof. Writing

$$S(t) = \sum_{k=1}^n c_k(t), \quad (3.6.6)$$

the equation is

$$c'_j = \frac{1}{2} \sum_{k=1}^{j-1} c_{j-k} c_k - S(t) c_j. \quad (3.6.7)$$

The idea is to solve (3.6.7) for an arbitrary function $S(t)$. The solution is then used in (3.6.6) to obtain an explicit solution for $S(t)$ and hence $c_j(t)$.

Define new variables $z(t)$ and $\phi_j(t)$ by

$$\frac{dz}{dt} = \frac{1}{2} \exp \left(- \int_0^t S(w) dw \right), \quad z(0) = 0, \quad (3.6.8)$$

$$\phi_j(z) = c_j(t) \exp \left(\int_0^t S(w) dw \right). \quad (3.6.9)$$

A calculation shows that

$$\frac{d\phi_j}{dz} = \sum_{k=0}^{j-1} \phi_k \phi_{j-k}, \quad \phi_1(0) = 1, \quad \phi_j(0) = 0, \quad j \geq 2. \quad (3.6.10)$$

Solving (3.6.10) gives

$$\phi_j(z) = z^{j-1}.$$

The consistency condition (3.6.6) is

$$S(z) = \exp\left(-\int_0^t S(w)dw\right) \sum_{k=1}^n z^{k-1},$$

so that

$$S(z) = 2\frac{dz}{dt} \sum_{k=1}^n z^{k-1}. \quad (3.6.11)$$

We introduce another variable $p(z)$ by

$$p = \frac{dz}{dt}.$$

From (3.6.8)

$$\frac{d^2z}{dt^2} = p\frac{dp}{dz} = -Sp.$$

Using this in (3.6.11) gives

$$\frac{dp}{dz} = -2p \sum_{k=1}^n z^{k-1}. \quad (3.6.12)$$

From (3.6.8), $p(0) = \frac{1}{2}$ so solving (3.6.12) with this data gives

$$p(z) = \frac{1}{2}e^{-f(z)},$$

where $f(z)$ is given in (3.6.4). Hence

$$\frac{dt}{dz} = 2e^{f(z)},$$

and using $z(0) = 0$ gives (3.6.5). This completes the proof.

From (3.6.5) we see that $z(t) \rightarrow \infty$ as $t \rightarrow \infty$. In order to find the large time behaviour of $c_j(t)$ we first have to study the asymptotics of $I(z)$ for large z . Integrating by parts in (3.6.5)

$$I(z) = \frac{2e^{f(z)}}{f'(z)} - \frac{2e^{f(0)}}{f'(0)} + 2 \int_0^z \frac{f''(w)e^{f(w)}}{(f'(w))^2} dw. \quad (3.6.13)$$

From this we expect $I(z)$ to behave like the first term on the right of (3.6.13). For large z ,

$$f'(z) = 2z^{n-1}(1 + o(1)), \quad (3.6.14)$$

so we expect $I(z) \sim z^{1-n}e^{f(z)}$ for large z .

Lemma 3.6.2.

$$\lim_{z \rightarrow \infty} \frac{I(z)}{z^{1-n}e^{f(z)}} = 1 \quad (3.6.15)$$

Proof: It is easier to use L'Hopitals rule to prove this rather than (3.6.13). Writing $D(z) = z^{1-n}e^{f(z)}$ we have that $D(z)$ and $I(z)$ tend to infinity as z tends to infinity. Also

$$\frac{I'(z)}{D'(z)} = \frac{2}{(1-n)z^{-n} + f'(z)z^{1-n}},$$

and the result follows from (3.6.14)

We use the information in the above result to calculate the decay rates of $(c_j(t))$.

Theorem 3.6.3. *For the initial data given by (3.6.2)*

$$\lim_{t \rightarrow \infty} t(\ln t)^{\frac{n-j}{n}} c_j(t) = \left(\frac{n}{2}\right)^{\frac{j-n}{n}} \quad (3.6.16)$$

Proof: Writing $z = z(t)$, from $I(z) = t$ and Lemma 3.6.2,

$$\exp(f(z) + (1 - n) \ln z) = t(1 + o(1)), \quad (3.6.17)$$

so that

$$f(z) + (1 - n) \ln z = \ln t + o(1).$$

From (3.6.4) and the above,

$$z = \left(\frac{n}{2}\right)^{1/n} (\ln t)^{1/n} (1 + o(1)). \quad (3.6.18)$$

Combining (3.6.17) and (3.6.18)

$$\begin{aligned} e^{f(z)} &= tz^{n-1}(1 + o(1)) \\ &= t \left(\frac{n}{2}\right)^{\frac{n-1}{n}} (\ln t)^{\frac{n-1}{n}} (1 + o(1)). \end{aligned}$$

Hence

$$e^{-f(z)} = t^{-1} \left(\frac{n}{2}\right)^{\frac{1-n}{n}} (\ln t)^{\frac{1-n}{n}} (1 + o(1)). \quad (3.6.19)$$

From formula (3.6.3) for $c_j(t)$, (3.6.18) and (3.6.19)

$$t (\ln t)^{\frac{n-j}{n}} c_j(t) = (z(\ln t)^{-1/n})^{j-1} \left(e^{-f(z)} t (\ln t)^{\frac{n-1}{n}} \right),$$

converges to

$$\left(\frac{n}{2}\right)^{\frac{j-1}{n}} \left(\frac{n}{2}\right)^{\frac{1-n}{n}} = \left(\frac{n}{2}\right)^{\frac{j-n}{n}}.$$

This completes the proof.

In Section 3.8 we study the $n = 2$ case of the coagulation equations which include the constant rate case. The calculations there will explain the origins of the $(\ln t)^{1/2}$ term in $c_1(t)$ in Theorem 3.6.3.

The next result shows that the rate of decay of the left hand side of (3.6.16) to its limit is very slow. Define γ_n by

$$\gamma_n = \left(\frac{n}{2}\right)^{\frac{1}{n}}.$$

Theorem 3.6.4.

$$\lim_{t \rightarrow \infty} (\ln t)^{\frac{1}{n}} \left(\gamma_n^{j-n} - t (\ln t)^{\frac{n-j}{n}} c_j(t) \right) = \gamma_n^{j-n-1}. \quad (3.6.20)$$

Proof: Using $c_j(t) = z^{j-1} e^{-f(z)}$ and $t = I(z)$ we have to find the limit of

$$(\ln t)^{\frac{1}{n}} \left(\gamma_n^{j-n} - I(z) z^{j-1} e^{-f(z)} (\ln t)^{\frac{n-j}{n}} \right). \quad (3.6.21)$$

From (3.6.18),

$$(\ln t)^{\frac{1}{n}} = \gamma_n^{-1} z (1 + o(1)). \quad (3.6.22)$$

Using this, (3.6.21) is equal to

$$\gamma_n^{-1} z (1 + o(1)) \left[\gamma_n^{j-n} - I(z) e^{-f(z)} z^{j-1} z^{n-j} (1 + o(1)) \right]$$

which may be written as

$$\gamma_n^{j-n-1} \left[z - I(z) e^{-f(z)} z^n \right] [1 + o(1)].$$

Hence it is sufficient to prove that

$$z - I(z)e^{-f(z)}z^n = \frac{ze^{f(z)} - I(z)z^n}{e^{f(z)}} = \frac{T(z)}{B(z)} \quad (3.6.23)$$

converges as $z \rightarrow \infty$. Since $e^{f(z)} \rightarrow \infty$ as $z \rightarrow \infty$, we can use L'Hopital's Rule to determine the limit. Using (3.6.4)

$$\begin{aligned} T'(z) &= e^{f(z)}(1 + 2z^n + 2z^{n-1} + o(z^{n-2})) - nz^{n-1}I(z) - 2z^n e^{f(z)} \\ &= e^{f(z)}(1 + 2z^{n-1} + o(z^{n-2}) - nz^{n-1}I(z)e^{-f(z)}). \end{aligned}$$

Using Lemma (3.6.2),

$$T'(z) = e^{f(z)}(1 + 2z^{n-1} + o(z^{n-2}) - n + o(1)).$$

Also,

$$B'(z) = 2e^{f(z)}(z^{n-1} + z^{n-2} + o(z^{n-3})).$$

Hence

$$\lim_{z \rightarrow \infty} \frac{T'(z)}{B'(z)} = 1,$$

so that

$$\lim_{z \rightarrow \infty} \frac{T(z)}{B(z)} = 1$$

and the result follows.

The $\ln t$ terms in (3.6.16) and in the decay rate results above, indicates that the

convergence in (3.6.16) may be slow. Figure 3.11 shows the graphs of

$$d_j(t) = \left(\frac{2}{n}\right)^{\frac{j-n}{2}} t (\ln(t))^{\frac{n-j}{n}} c_j(t) \quad (3.6.24)$$

for the numerical solution of (3.6.1) for the case $n = 4$. By Theorem 3.6.3, each of the expressions in (3.6.24) should converge to 1 as $t \rightarrow \infty$. Figure 3.11 shows that for $t = 10^5$, $d_1(t)$ is close to 1 while d_2, d_3, d_4 are far from their limit values.

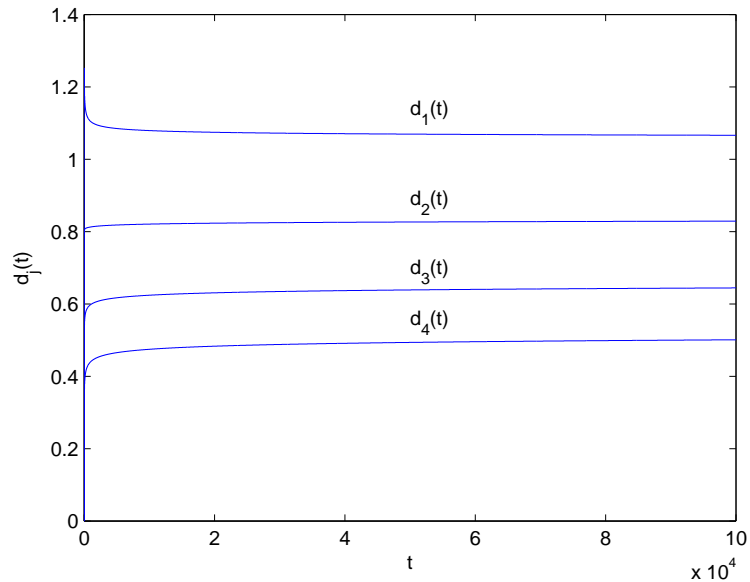


Figure 3.11: Theorem (3.6.3) when $n = 4$ with different j

3.7 The modified system

In this section we make a change of variables which will focus on the possible $O(t^{-1})$ large time behaviour of solutions to the coagulation equations (3.5.1). The resulting

equations will be called the modified system. The change of variables was introduced in [11] in an attempt to study gelation for the case in which $a_{jk} = r_j r_k$. We will assume $a_{jk} > 0$ for all j and k throughout this section.

Let $c = (c_j(t))$ be a solution of (3.6.1). We use a new time scale

$$\tau = \tau(t) = \ln(t + 1), \quad (3.7.1)$$

and new variables $y_j(\tau)$ where

$$y_j(\tau) = (1 + t)c_j(t). \quad (3.7.2)$$

We note from (3.7.1) that the initial time $t = 0$ corresponds to the initial time $\tau = 0$.

The transform changes the original equations into another autonomous system given by

$$\frac{dy_j}{d\tau} = y_j + \frac{1}{2} \sum_{k=1}^{j-1} a_{j-k,k} y_{j-k} y_k - y_j \sum_{k=1}^n a_{jk} y_k. \quad (3.7.3)$$

The initial data for the equations is nonnegative.

The above construction also allows us to transfer results for the coagulation equations (3.6.1) to the new system. Hence we have that global existence and uniqueness hold as well as positivity of solutions.

The new system has certain advantages over (3.6.1), for example it contains some linear terms and there is the possibility of equilibrium solutions. Suppose for example that we could prove for some component that

$$y_j(\tau) = e^{-\lambda\tau} (L + o(1)) \quad \text{as } \tau \rightarrow \infty,$$

for some $L > 0$ and $\lambda \geq 0$. By (3.7.1) and (3.7.2) it would follow that

$$c_j(t) = t^{-1+\lambda}(L + o(1)) \quad \text{as } t \rightarrow \infty.$$

More generally we have that

(i) $y_j(\tau) \rightarrow 0$ as $\tau \rightarrow \infty$ if and only if $c_j(t) = o(t^{-1})$ as $t \rightarrow \infty$.

(ii) $y_j(\tau)$ is bounded as $\tau \rightarrow \infty$ if and only if $c_j(t) = O(t^{-1})$ as $t \rightarrow \infty$.

The next result which is proved in [11] shows that all components of y are bounded and that we cannot have all components of y tending to zero.

Theorem 3.7.1. *Let y be a nonzero solution of (3.7.3). Then y is bounded and bounded away from zero as $\tau \rightarrow \infty$.*

3.8 Analysis of the $n=2$ case.

We study the coagulation equation with $n = 2$. For this case there are three parameters, a_{11} , a_{12} , a_{22} . By scaling time we can fix $a_{11} = 1$ and we write $a_{12} = \alpha$, $a_{22} = \beta$.

The modified system (3.7.3) is

$$\begin{aligned} \frac{dy_1}{d\tau} &= y_1 - y_1^2 - \alpha y_1 y_2, \\ \frac{dy_2}{d\tau} &= y_2 + \frac{1}{2} y_1^2 - \alpha y_1 y_2 - \beta y_2^2. \end{aligned} \tag{3.8.1}$$

We will study equilibrium solutions to these equations and their stability. Even though there are only two parameters we will show that there is a range of possible decay rates. There are two possible forms of equilibria for (3.8.1), depending on $y_1 = 0$ or $y_1 \neq 0$. We begin by studying solutions with $y_1 = 0$.

Case 1 : Equilibria with $y_1 = 0$.

We study the equilibrium solution

$$\bar{y} = (0, \beta^{-1}). \quad (3.8.2)$$

The linearised matrix at \bar{y} is given by

$$\begin{bmatrix} 1 - \alpha\beta^{-1} & 0 \\ -\alpha\beta^{-1} & -1 \end{bmatrix}$$

with eigenvalues $1 - \alpha\beta^{-1}$ and -1 . It follows that the equilibrium \bar{y} is asymptotically stable if $\alpha > \beta$ and unstable if $\alpha < \beta$. If $\alpha = \beta$ then there is a zero eigenvalue and further calculations are needed to determine stability.

Suppose $\alpha > \beta$. We determine the rate of decay to \bar{y} . Define p by

$$p = \min(\alpha\beta^{-1} - 1, 1), \quad (3.8.3)$$

and suppose $\alpha\beta^{-1} \neq 2$. Then for solutions starting near \bar{y} we have that

$$\lim_{\tau \rightarrow \infty} e^{p\tau} y_1(\tau) = L,$$

while

$$\lim_{\tau \rightarrow \infty} y_2(\tau) = \beta^{-1},$$

with $L \neq 0$ in general. We omit the case $\alpha\beta^{-1} = 2$ since in this case the linearised matrix would contain a Jordan block and asymptotic behaviour would need to be

modified. We now translate this information about $y(\tau)$ to obtain the asymptotic behaviour of solutions to the coagulation equations.

Lemma 3.8.1. *Suppose that $\alpha > \beta$ and that $\alpha\beta^{-1} \neq 2$. Let c be a solution with initial data close to $(0, \beta^{-1})$. Then with p defined by (3.8.3)*

$$\lim_{t \rightarrow \infty} t^{p+1} c_1(t) = L. \quad (3.8.4)$$

$$\lim_{t \rightarrow \infty} t c_2(t) = \beta^{-1}. \quad (3.8.5)$$

Figure 3.12 shows the graph of $tc_2(t)$ for the case $\alpha = 6$ and $\beta = 2$. As predicted,

$$\lim_{t \rightarrow \infty} tc_2(t) = \beta^{-1} = 0.5.$$

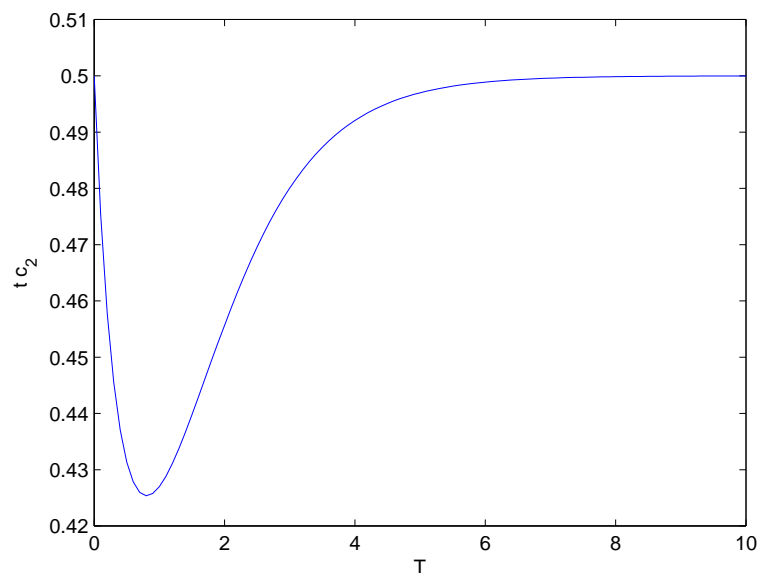


Figure 3.12: Graph of $tc_2(t)$. The initial condition is $c_1(0) = 0.1$, $c_2(0) = 0.5$.

For the case $\alpha > \beta$ we will show later in this section that there is a region Q in $\alpha - \beta$ space (with $\alpha > \beta$) such that :

- (i) if (α, β) is in Q then (3.8.1) does not have any additional equilibrium solutions.
- (ii) if (α, β) does not lie in Q then there are equilibriums solution to (3.8.1) with $y_1 \neq 0$.

For case (i) with (α, β) in Q we would expect that Lemma 3.8.1 would apply for all initial data .

For case (ii) with (α, β) not in Q the asymptotic behaviour will depend on the initial data. For initial data in some region which includes the equilibrium \bar{y} given by (3.8.2), the asymptotics described in Lemma 3.8.1 would apply. For certain initial data outside this region, y would be attracted to one of the equilibria with $y_1 \neq 0$ so that

$$\lim_{t \rightarrow \infty} t c_1(t) = L > 0. \quad (3.8.6)$$

This completes our study of equilibrium (3.8.2) for the case $\alpha > \beta$.

If $\beta > \alpha$ then \bar{y} is unstable. We will show later in this section that if $\beta > \alpha$ then there is a unique equilibrium (y_1, y_2) with $y_1 > 0$.

We now study the stability of \bar{y} when $\alpha = \beta$. In this case the linearised problem has eigenvalues 0 and -1 so we need to do a centre manifold calculation to determine stability.

Lemma 3.8.2. *Assume $\alpha = \beta$ for (3.8.1)*

- (a) *If $\alpha > 1$ then \bar{y} is unstable.*

(b) If $\alpha < 1$ then \bar{y} is asymptotically stable and for most initial data close to \bar{y} ,

$$\lim_{\tau \rightarrow \infty} \tau y_1(\tau) = (1 - \alpha)^{-1}. \quad (3.8.7)$$

(c) If $\alpha = 1$ then \bar{y} asymptotically stable and for most initial data close to \bar{y}

$$\lim_{\tau \rightarrow \infty} \tau^{1/2} y_1(\tau) = 1. \quad (3.8.8)$$

Using the transformation given by (3.7.1) and (3.7.2) gives the following results.

Lemma 3.8.3. *Assume $\alpha = \beta$. For the coagulation equations with initial data close to \bar{y} :*

(i) if $\alpha > 1$ then

$$\lim_{t \rightarrow \infty} t \ln t c_1(t) = (1 - \alpha)^{-1}; \quad (3.8.9)$$

(ii) if $\alpha = 1$ then

$$\lim_{t \rightarrow \infty} t (\ln t)^{1/2} c_1(t) = 1, \quad (3.8.10)$$

$$\lim_{t \rightarrow \infty} t c_2(t) = 1. \quad (3.8.11)$$

Figures (3.13) - (3.16) show the results of some numerics for the case $\alpha = \beta$. Figure (3.13) shows that (3.8.7) holds when $\alpha < 1$. The remaining figures are for the cases $\alpha = \beta = 1$.

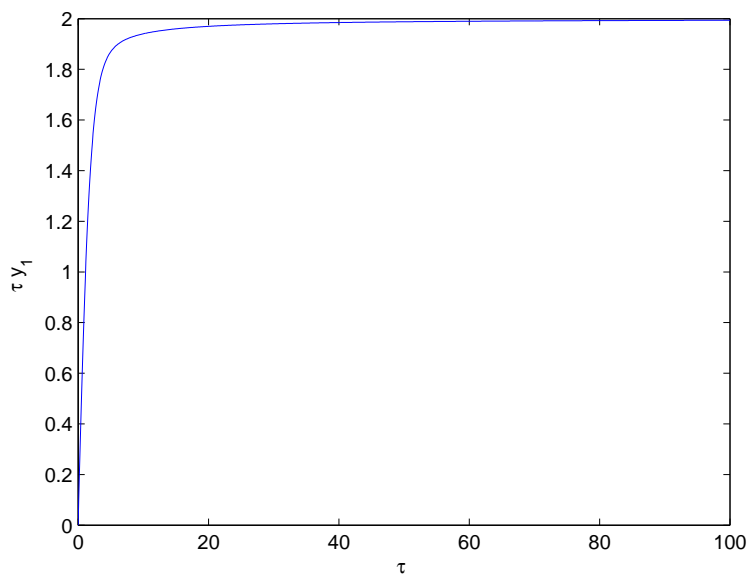


Figure 3.13: Behaviour of $\tau y_1(\tau)$ when $\alpha = 0.5 = \beta$. The initial conditions are $c_1(0) = 0.1$, $c_2(0) = 0.5$.

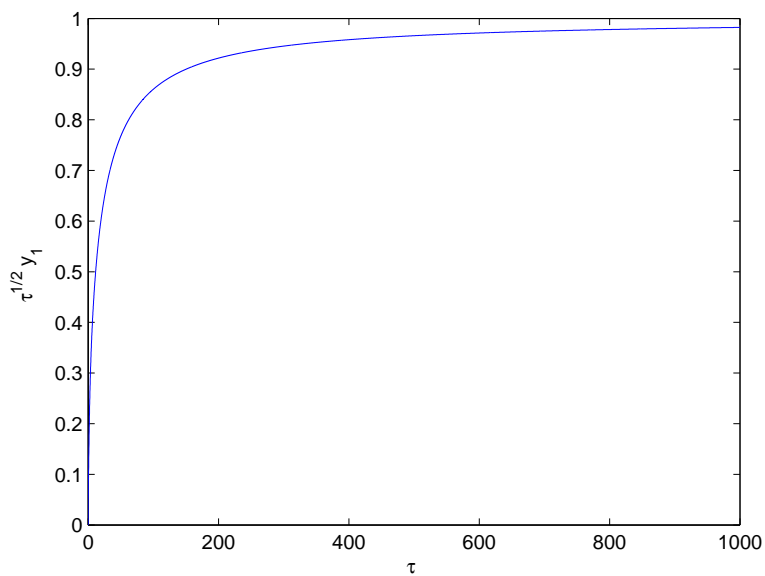


Figure 3.14: Graph of $\tau y_1(\tau)$ when $\alpha = \beta = 1$, $c_1(0) = 0.1$, $c_2(0) = 0.5$.

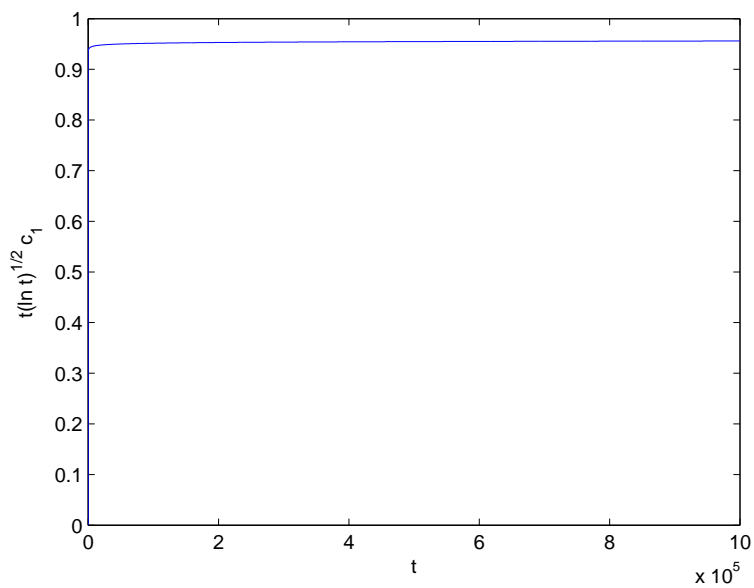


Figure 3.15: Graph of $t(\ln t)^{1/2} c_1(t)$ when $\alpha = \beta = 1, c_1(0) = 1, c_2(0) = 0$.

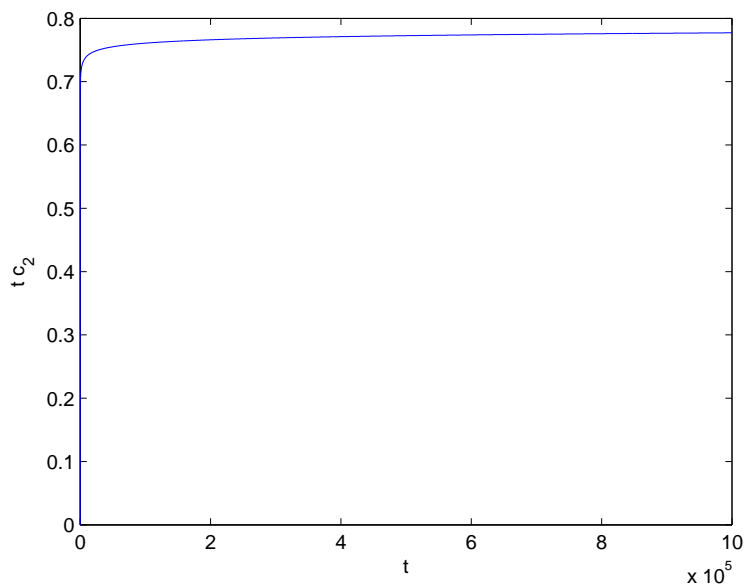


Figure 3.16: Graph of $t c_2(t)$ when $\alpha = \beta = 1, c_1(0) = 1, c_2(0) = 0$.

We note that the case $\alpha = \beta = 1$ corresponds to constant coagulation rates $a_{jk} = 1$ with $n = 2$. Putting $n = 2$ in (3.6.16) we see that Theorem 3.6.3 predicts the same large time behaviour as (3.8.10) and (3.8.11). The calculations in Lemma 3.8.2 explain the delicate asymptotics near $\alpha = 1$. The centre manifold calculations will show that the asymptotic behaviour of $\bar{y}_1(\tau)$ is determined by the scalar equation

$$\frac{du}{d\tau} = -\frac{u^3}{2}(1 + O(u)),$$

so that

$$\lim_{\tau \rightarrow \infty} \tau^{1/2} u(\tau) = 1,$$

which explains the $(\ln t)^{1/2}$ term in (3.8.10).

Proof of Lemma 3.8.2.

We first translate the equilibrium $(0, \alpha^{-1})$ to the origin via the change of variables $y_1 = y_1$, $y_2 = z + \beta^{-1}$. Denoting the derivative with respect to τ by a prime, equation (3.8.1) becomes

$$y_1' = -y_1^2 - \alpha y_1 z, \tag{3.8.12}$$

$$z' = -y_1 - z + \frac{1}{2} y_1^2 - \alpha y_1 z - \beta z^2.$$

The linearised matrix about the equilibrium $(0, 0)$ is

$$\begin{bmatrix} 0 & 0 \\ -1 & -1 \end{bmatrix}.$$

To apply centre manifold theory we have to put this in diagonal form. Using the

variables y_1, w with $w = y_1 + z$ we obtain

$$y_1' = N_1(y_1, w), \quad w' = -w + N_2(y_1, w), \quad (3.8.13)$$

where

$$N_1(y_1, w) = (\alpha - 1) y_1^2 - \alpha y_1 w, \quad (3.8.14)$$

$$N_2(y_1, w) = N_1(y_1, w) + \frac{1}{2} y_1^2 - \alpha w(w - y_1). \quad (3.8.15)$$

It follows from the theory given in Section 1.5 that there is a centre manifold $w = h(y_1)$ with $h(y_1) = O(y_1^2)$ as $y_1 \rightarrow 0$. The equation on the centre manifold is

$$u' = N_1(u, h(u)) = (\alpha - 1) u^2 - \alpha u h(u). \quad (3.8.16)$$

This equation describe the solution of the full system (3.8.13) except for an exponentially small term, which is of order $e^{-\tau}$.

Since we only know that $h(u) = O(u^2)$ we need a better approximation to $h(u)$ in order to describe solutions to (3.8.16), for the case $\alpha = 1$. For $\alpha \neq 1$ we have that

$$u' = (\alpha - 1) u^2 + O(u^3). \quad (3.8.17)$$

If $\alpha > 1$ then $u = 0$ is unstable for (3.8.17). This proves part (a) of Lemma 3.8.2.

Suppose now that $\alpha < 1$. Then $u = 0$ is asymptotically stable which proves that

\bar{y} is also asymptotically stable. Solving (3.8.17) shows that if $u(0) > 0$ then

$$\lim_{\tau \rightarrow \infty} \tau u(\tau) = (1 - \alpha)^{-1}.$$

Equation (3.8.13) also has a stable manifold on which solutions decay to zero like $e^{-\tau}$.

The stable manifold corresponds to taking $u(0) = 0$ for (3.8.17). It follows that for most initial data,

$$\lim_{\tau \rightarrow \infty} \tau y_1(\tau) = (1 - \alpha)^{-1}, \quad (3.8.18)$$

which proves part (b).

We now take $\alpha = 1$ so that $u' = O(u^3)$. We use theory given in Section 1.5 to calculate the quadratic term in $h(u)$.

Let $\phi : \mathbf{R} \rightarrow \mathbf{R}$ with $\phi(u) = O(u^2)$ and define $(M\phi)(u)$ by

$$(M\phi)(u) = \phi'(u) N_1(u, \phi(u)) + \phi(u) - N_2(u, \phi(u)).$$

If ϕ is such that $(M\phi)(u) = O(u^q)$, $q \geq 2$, then we would have $h(u) = \phi(u) + O(u^q)$.

Note that for the case $\alpha = 1$ we have that $N_1(u, \phi(u)) = -u\phi(u)$. Let

$$\phi(u) = \frac{u^2}{2}.$$

Then

$$\phi'(u) N_1(u, \phi(u)) = O(u^4),$$

$$\phi(u) - N_2(u, \phi(u)) = O(u^3).$$

It follows that $(M\phi)(u) = O(u^3)$ so that

$$h(u) = \frac{u^2}{2} + O(u^3),$$

and the equation on the centre manifold is

$$u' = -\frac{u^3}{2} + O(u^4).$$

Part (c) of Lemma 3.8.2 follows by solving the above equation and this completes the proof.

The proof of Lemma 3.8.3 follows from the previous Lemma, the transformed variables (3.7.1) and (3.7.2) and the fact that $y_2(\tau)$ converges to the equilibrium point 1.

This completes our analysis of equilibria with $y_1 = 0$. The main results are Lemma 3.8.1 and Lemma 3.8.3.

Case 2 : Equilibria with $y_1 \neq 0$.

Let (y_1, y_2) be an equilibrium solution of (3.8.1) with $y_1 \neq 0$. From the second equation in (3.8.1) we have that $y_2 \neq 0$ and from the first,

$$y_2 = \alpha^{-1}(1 - y_1). \tag{3.8.19}$$

Substituting this into the second equation in (3.8.1) shows that y_1 must be a solution

of the quadratic equation

$$\mathcal{G}(y_1) = \left(\frac{3\alpha^2 - 2\beta}{2} \right) y_1^2 + (2\beta - \alpha - \alpha^2)y_1 + \alpha - \beta = 0, \quad (3.8.20)$$

with $0 < y_1 < 1$. We call a solution of $\mathcal{G}(y_1) = 0$ admissible if $0 < y_1 < 1$. The number of such solutions will depend on α and β .

The curve

$$2\beta = 4\alpha - \alpha^2 - 1 \quad , \quad 1 < \alpha < 2 + \sqrt{3}, \quad (3.8.21)$$

divides the region $\alpha > \beta$ into points Q which are on the left of this curve and points S on the right of this curve. The other region P is $\beta > \alpha$.

In detail,

$$P = \{(\alpha, \beta) : \beta > \alpha > 0\},$$

$$Q = \{(\alpha, \beta) : \alpha > \beta > 0 \text{ and } 2\beta < 4\alpha - \alpha^2 - 1\},$$

$$S = \{(\alpha, \beta) : \alpha > \beta > 0 \text{ and } 2\beta > 4\alpha - \alpha^2 - 1\}.$$

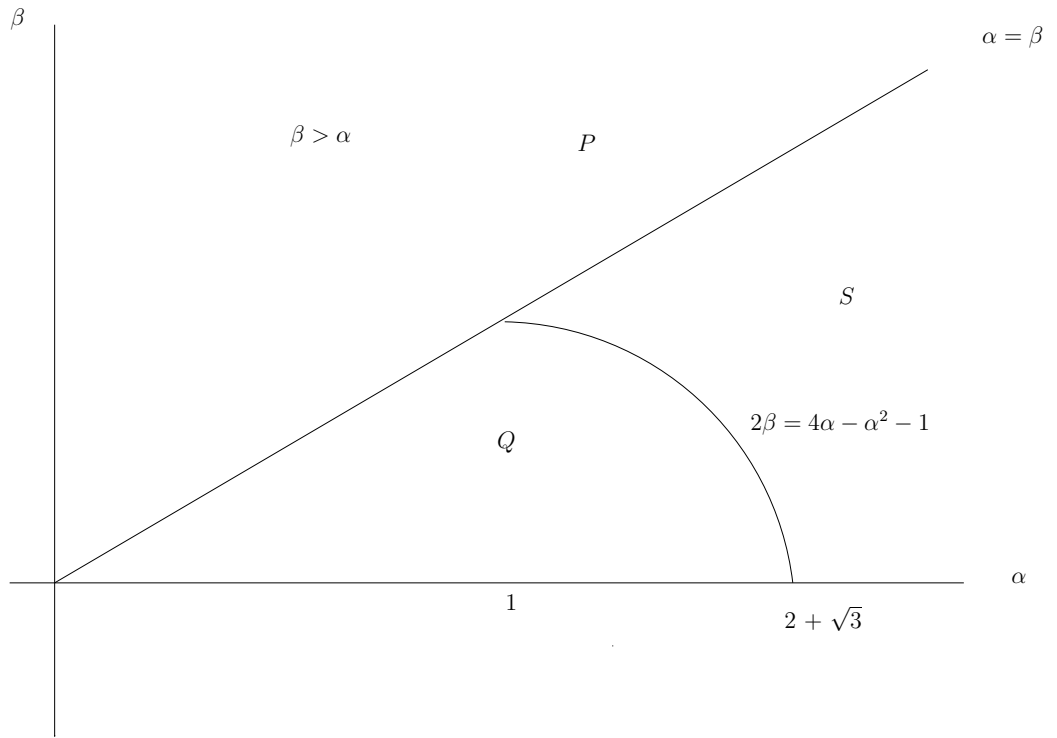


Figure 3.17: Regions P, Q and S .

We note that for the curve given by (3.8.21) we have that $\beta'(1) = 1$ so that it is tangent to the curve $\alpha = \beta$ at $\alpha = 1$. Figure (3.17) shows that $\alpha - \beta$ plane divided into the regions P, Q and S .

The next result gives the number of equilibrium solutions with $y_1 \neq 0$ in the various regions.

Lemma 3.8.4. (a) For (α, β) in P there is a unique equilibrium with $y_1 \neq 0$.

(b) If (α, β) is in Q then there are no equilibrium solutions with $y_1 \neq 0$.

(c) For (α, β) in S there are two distinct equilibrium solutions with $y_1 \neq 0$.

(d) On the boundary of Q and S given by (3.8.21) there is a unique solution with

$y_1 \neq 0$ given by

$$y_1 = \frac{\alpha - 1}{2\alpha - 1}.$$

The solution is double in the sense $\mathcal{G}(y_1) = \mathcal{G}'(y_1) = 0$.

(e) On the boundary line $\alpha = \beta$ there are no equilibrium solutions with $y_1 \neq 0$ for $\alpha \leq 1$ and a unique one for $\alpha > 1$ given by

$$y_1 = \frac{2(\alpha - 1)}{3\alpha - 2}.$$

Proof of Lemma (3.8.4) part (a)

Assume $\beta > \alpha > 0$. We have that

$$\mathcal{G}(0) = \alpha - \beta < 0 \quad , \quad \mathcal{G}(1) = \frac{\alpha^2}{2} > 0,$$

so there is at least one admissible solution. If $3\alpha^2 - \beta \neq 0$ then \mathcal{G} is quadratic so it is unique. If $3\alpha^2 - \beta = 0$ then the equation is linear with solution

$$y_1 = \frac{3\alpha - 2}{4\alpha - 2}. \tag{3.8.22}$$

This solution is admissible since $\beta > \alpha$ and $3\alpha^2 = 2\beta$ implies that $\alpha > 2/3$.

Proof of Lemma 3.8.4 parts(b), (c) and (d)

We begin by showing that there are no admissible solutions in various regions in $\alpha - \beta$ space. We first show that there are no admissible solution in the region

$$\alpha > \beta \quad \text{and} \quad 2\beta > 3\alpha^2.$$

The above inequalities imply that $\alpha < 2/3$ so this region lies in the region Q . The nonexistence of admissible solution follows from $\mathcal{G}(0) > 0$, $\mathcal{G}(1) > 0$ and that the coefficient of y_1^2 is negative.

Assume now that $\alpha > \beta$. Then

$$\mathcal{G}(0) = \alpha - \beta > 0, \quad Q(1) = \frac{\alpha^2}{2} > 0.$$

A calculation shows that $Q'(1) = 2\alpha^2 - \alpha$ so there are no admissible solutions if $\alpha \leq 1/2$. Also, since $\mathcal{G}(0)$ and $\mathcal{G}(1)$ are positive, there will not be any admissible solution. Since $\mathcal{G}(0) > 0$, $\mathcal{G}(1) > 0$ and $Q'(1) > 0$, there are no admissible solutions if $\mathcal{G}'(0) > 0$, that is, if $\alpha + \alpha^2 > 2\beta$.

Combining this information, we have shown that there are no admissible solutions for various values of α and β . Hence for the rest of the proof of parts (b), (c) and (d) we may assume that

$$\alpha > \beta, \quad \alpha > 1/2, \quad 3\alpha^2 > 2\beta \quad \text{and} \quad \alpha + \alpha^2 > 2\beta. \quad (3.8.23)$$

The idea behind the rest of the proof is as follows. Since the coefficient of y_1^2 is positive, the quadratic will have a minimum at $y_1 = m$. The calculation of m and the minimum value $\mathcal{G}(m)$ will lead to conditions for the existence of admissible solutions.

The quadratic has a minimum at $y_1 = m$ given by

$$m = \frac{\alpha + \alpha^2 - 2\beta}{3\alpha^2 - 2\beta}$$

which is positive by (3.8.23). Also,

$$(3\alpha^2 - 2\beta)(1 - m) = 2\alpha^2 - \alpha > 0$$

since $\alpha > 1/2$. The minimum value $\mathcal{G}(m)$ is given by

$$2(3\alpha^2 - 2\beta)\mathcal{G}(m) = \alpha^2(4\alpha - \alpha^2 - 1 - 2\beta).$$

For admissible solution to exist we require $\mathcal{G}(m) \leq 0$.

so that

$$2\beta \geq 4\alpha - \alpha^2 - 1. \tag{3.8.24}$$

Combining this inequality with the inequality $\alpha + \alpha^2 > 2\beta$ from (3.8.23) gives

$$\alpha + \alpha^2 \geq 4\alpha - \alpha^2 - 1,$$

so that

$$2\alpha^2 - 3\alpha + 1 = 2(\alpha - 1)(\alpha - 1/2) \geq 0.$$

Since we have $\alpha > 1/2$ this shows that $\alpha \geq 1$. If $\alpha = 1$ then (3.8.24) would imply that $\beta \geq 1 = \alpha$ which contradicts $\alpha > 0$. This shows that we must have $\alpha > 1$. Since $\beta > 0$ we must have $4\alpha - \alpha^2 - 1 > 0$. Using $4\alpha - \alpha^2 - 1 = 3 - (\alpha - 2)^2$, leads to the additional inequality for the boundary curve between Q and S ,

$$\alpha < 2 + \sqrt{3}.$$

If (3.8.21) holds then $\mathcal{G}(m) = \mathcal{G}'(m) = 0$ and

$$m = \frac{2\alpha^2 - 3\alpha + 1}{4\alpha^2 - 4\alpha + 1} = \frac{\alpha - 1}{2\alpha - 1},$$

as required.

Proof of Lemma 3.8.4 parts(d)

If $\alpha = \beta$ then the solutions of $\mathcal{G}(y_1) = 0$ are $y_1 = 0$ and

$$y_1 = \frac{2(\alpha - 1)}{3\alpha - 2},$$

with

$$1 - y_1 = \frac{\alpha}{3\alpha - 2}.$$

This solution is admissible if and only if $\alpha > 1$ and the result follows. This completes the proof of Lemma 3.8.4.

Example 3.8.1

In [11] the product kernel $a_{j,k} = r_j r_k$ was considered with (r_j) a strictly increasing sequence. It was proved for the modified equations, that for general any n there was a unique equilibrium with all components positive. We work out the details for $n = 2$. Since $a_{1,1} = 1, r_1 = 1$. Also, $a_{12} = \alpha = r_2$ so $\beta = a_{22} = r_2^2 = \alpha^2$. Since $r_2 > r_1$ we have that

$$\beta = \alpha^2, \alpha > 1.$$

This shows that (α, β) is in region P so by Lemma 3.8.4 there is a unique equilib-

rium with $y_1 \neq 0$. A calculation shows that

$$\alpha y_1 = 1 - \alpha + \sqrt{D}, \quad (3.8.25)$$

where

$$D = (\alpha - 1)^2 + 2\alpha(\alpha - 1).$$

Since $D > \alpha - 1$ we have $y_1 > 0$. Also,

$$\alpha(1 - y_1) = \frac{3\alpha^2}{2\alpha - 1 + \sqrt{D}} > 0,$$

so that y_1 is admissible.

It would be interesting to study the local stability of the equilibria described in Lemma 3.8.4. However, the algebra becomes very complicated so we study some special cases.

For the case $\beta > \alpha$ which is region P in Lemma 3.8.4, we have that the equilibrium $(0, \beta^{-1})$ is unstable. We would expect that most solutions to (3.8.1) would converge to the equilibrium with $y_1 > 0$. We will prove below that this equilibrium is locally stable for the special cases

$$(a) \beta = \alpha^2, \alpha > 1 \quad (b) 2\beta = 3\alpha^2, \alpha > \frac{2}{3}.$$

If $\alpha < \beta$ then the equilibrium $(0, \beta^{-1})$ is locally stable. If (α, β) is in Q then there are no other equilibrium solutions and we would expect all solutions to (3.8.1) converge to $(0, \beta^{-1})$. The line $\alpha = \beta$ with $\alpha < 1$ forms parts of the boundary of Q .

In Lemma 3.8.2 part (b) we proved that $(0, \beta^{-1})$ is locally stable on this line.

If $\alpha < \beta$ and (α, β) is in S then there are two additional equilibrium solutions. We would expect one of these, say (\bar{y}_1, \bar{y}_2) to be stable while the other is unstable. For this case we would expect some solutions to converge to $(0, \beta^{-1})$ while others would converge to (\bar{y}_1, \bar{y}_2) .

The line $\alpha = \beta$ with $\alpha > 1$ forms part of the boundary between P and S . We prove below that on this line the equilibrium with $y_1 > 0$ is stable.

Suppose we have an equilibrium with $y_1 \neq 0$ so that y_1 is a solution of the quadratic equation given by (3.8.20). A calculation shows that λ is an eigenvalue of the linearised problem if

$$\lambda^2 + B\lambda + C = 0,$$

with

$$B = y_1(\alpha - 2\beta\alpha^{-1} + 1) + 2\beta\alpha^{-1} - 1,$$

$$C = y_1^2(\alpha - 2\beta\alpha^{-1}) + \alpha y_1(2y_1 - 1) + (2\beta\alpha^{-1} - 1)y_1.$$

We prove that the real part of λ is negative in the examples below by showing that $B > 0$ and $C > 0$ in each case. This proves that the equilibrium with $y_1 > 0$ is locally stable in each of the examples.

Example 3.8.1 continued

For this case $\beta = \alpha^2$ and $\alpha > 1$. We show that the equilibrium with $y_1 > 0$ is stable. For this case

$$B = (1 - \alpha)y_1 + 2\alpha - 1.$$

Since $y_1 < 1$,

$$B > y_1(2\alpha - 1 + 1 - \alpha) = \alpha y_1 > 0.$$

Also,

$$y_1^{-1}C = \alpha y_1 + \alpha - 1.$$

Using (3.8.24)

$$y_1^{-1}C = 1 - \alpha + \sqrt{D} + \alpha - 1 = \sqrt{D} > 0$$

and this proves the stability.

Example 3.8.2

Suppose $3\alpha > 2$ and that $3\alpha^2 = 2\beta$. It follows that $\beta > \alpha$ so the parameters are in region P . For this case the quadratic equation (3.8.20) reduces to a linear equation and

$$(2\alpha - 1)y_1 = \frac{3\alpha - 2}{2}.$$

Using this ,

$$B = (1 - 2\alpha)y_1 + 3\alpha - 1 = \frac{3\alpha}{2} > 0.$$

Also,

$$y_1^{-1}C = 2\alpha - 1 > 0,$$

which proves stability.

Example 3.8.3

We consider the case $\alpha = \beta$ with $\alpha > 1$. In part(b) of Lemma 3.8.2 we proved

that the equilibrium $(0, \beta^{-1})$ is unstable on this line. In part(e) of Lemma 3.8.4 we proved that there is a unique equilibrium with $y_1 > 0$ given by

$$y_1 = \frac{2(\alpha - 1)}{3\alpha - 2}. \quad (3.8.26)$$

We prove that this equilibrium is locally stable. Using $\alpha = \beta$,

$$B = (\alpha - 1)y_1 + 1.$$

Since $y_1 < 1$,

$$B > y_1(1 + \alpha - 1) = \alpha y_1 > 0.$$

Also, using (3.8.26)

$$y_1^{-1}C = (3\alpha - 2)y_1 + 1 - \alpha = \alpha - 1 > 0$$

and this proves the stability result.

Chapter 4

A model for the treatment of Alzheimer's disease

4.1 Introduction

Alzheimer's disease is the most common form of dementia and is a major cause of death in the elderly. The causes and progression of the disease are not yet understood. One theory, the amyloid hypothesis [38], is one of the main ideas used to explain the damage that is done in the brain.

A protein fragment, amyloid beta ($A\beta$), is often found in the brain plaques of Alzheimer's disease patients. The amyloid hypothesis is that ($A\beta$) accumulation is the primary event in the development of the disease. The hypothesis is that there is either a fault with the over production of ($A\beta$) or with the mechanisms that remove ($A\beta$) from the brain (or possibly both).

One possible treatment is to try and lower ($A\beta$) production so that the total level of ($A\beta$) in the brain is below the critical concentration. One method is to use a

drug that interferes with the enzymes that create $(A\beta)$ from the amyloid precursor protein [38].

Polymers are macromolecules built up from linking a large number of smaller molecules which are termed monomers. The reactions by which the monomers combine is called polymerization.

In this chapter we study a mathematical model of the kinetics of $(A\beta)$ accumulation in the brain [8, 9]. The model includes the production and loss of $(A\beta)$ monomers and the elongation and fragmentation of polymers by monomer aggregation and monomer break-off. The resulting equations are of Becker-Doring type with the addition of loss and production terms.

We follow the papers in [8], [9] by studying the impact of production inhibitors on the total amount of $(A\beta)$ density (called the $(A\beta)$ burden). There are two main areas of interest:

- (i) Reduction in the production rate. This leads to the decay, in time, to a new reduced $(A\beta)$ burden.
- (ii) Looking at what happens when the treatment ends. For this case, the production rate is increased and after a time the $(A\beta)$ burden returns to a higher level.

There are four parameters in our model and they are all related to chemical time scales, that is, fractions of a second. However the time scales involved in the treatments (i) and (ii) are large, and are measured in months and years. The aim is to derive a formula depending on the parameters which predicts the rate of the decay.

The previous work [8], [9] only considered numerical solutions to the differential equations. In Section 4.3 we begin our mathematical study of the model by proving

the existence of a positive solution.

In Section 4.4 we find the unique equilibrium solution and prove its stability by means of a Lyapunov function. We also derive a formula for the $(A\beta)$ burden and show that it depends in a critical way on the polymerization ratio r . This quantity r depends on all four parameters in the problem.

In Section 4.5 we describe some numerics which model the treatment (i) and (ii) above. Finally, in Section 4.6 we derive our formula for the decay rate and check it against numerical solutions to the full equations.

4.2 A modified Becker - Döring equation

Our model tracks the dynamics of clusters of $(A\beta)$ monomers. Let $c_k(t)$ be the concentration of clusters consisting of k molecules at time t . The maximum cluster size is N . The differential equations give the evolution of these concentrations and are given by

$$\begin{aligned} \dot{c}_1 &= q - \alpha c_1 - W_1 - \sum_{k=1}^{N-1} W_k, \\ \dot{c}_k &= W_{k-1} - W_k, \quad 2 \leq k \leq N-1, \\ \dot{c}_N &= W_{N-1}, \end{aligned} \tag{4.2.1}$$

where

$$\begin{aligned} W_1 &= \beta c_1^2 - \frac{f}{2} c_2, \\ W_k &= \beta c_1 c_k - f c_{k+1} \quad k \geq 2, \end{aligned} \tag{4.2.2}$$

and all the parameters α , β , f and q are positive. We assume throughout this chapter that the initial data for (4.2.1) is nonnegative so that

$$c_k(0) \geq 0 \quad \text{for } 1 \leq k \leq N.$$

Typical values of the parameters are (using the time unit of days)

$$q = 8.81 \times 10^{-7}, \quad \alpha = 24, \quad \beta = 7.776 \times 10^6, \quad f = 0.3396. \tag{4.2.3}$$

and the number of equations is $N = 500$. These values will be used throughout this chapter.

4.3 Existence and positivity of solution

We begin our study of (4.2.1) by proving the existence of a positive solution for all $t \geq 0$. We let $c = (c_1, c_2, \dots, c_N)$.

Lemma 4.3.1. *Let c be a solution of (4.2.1) on some interval $[0, T)$, $T > 0$. Then $c_k(t) > 0$ for all k .*

Proof:

We first prove that $c_1(t) > 0$ for all $t \in (0, T)$. The equation for c_1 can be written as

$$\begin{aligned} c_1' + \phi(t)c_1 &= h(t), \\ \phi(t) &= 2\beta c_1 + \alpha + \sum_{k=2}^{N-1} \beta c_k, \\ h(t) &= q + \frac{f}{2}c_2 + f \sum_{k=1}^{N-1} c_{k+1}. \end{aligned}$$

Hence

$$c_1(t) \exp\left(\int_0^t \phi(s)ds\right) = c_1(0) + \int_0^t \exp\left(\int_0^s \phi(y)dy\right) h(s)ds.$$

Since $h(s) \geq q > 0$ for all s it follows that $c_1(t) > 0$ for $t \in (0, T)$.

Suppose for contradiction, $c_k(\tau) = 0$ for some $\tau \in (0, T)$ and $2 \leq k \leq N$. From the equation for c_N ,

$$(c_N e^{ft})' = \beta c_1 c_{N-1} e^{ft}.$$

Hence if $c_N(\tau) = 0$ then

$$0 = c_N(0) + \beta \int_0^\tau c_1(s) c_{N-1}(s) e^{fs} ds.$$

In particular, since $c_1(s) > 0$ we must have $c_{N-1}(\tau) = 0$.

From the equation for c_k , $2 \leq k \leq N - 1$

$$c_k' + \phi(t)c_k = h_k(t),$$

$$\phi(t) = f + \beta c_1,$$

$$h_k(t) = \beta c_1 c_{k-1} + f c_{k+1}, \quad 3 \leq k \leq N - 1,$$

$$h_2(t) = \beta c_1^2 + \frac{f}{2} c_3.$$

Hence if $c_k(\tau) = 0$ then

$$0 = c_k(0) + \int_0^\tau \exp\left(\int_0^s \phi(y) dy\right) h_k(s) ds.$$

It follows that we must have $c_{k-1}(\tau) = 0$.

We have shown that in all cases, $c_1(\tau) = 0$ which is a contradiction. This complete the proof.

Lemma 4.3.2. *Let c be a solution of (4.2.1) on $[0, T]$ and let (g_k) be a constant sequence.*

Then

$$\sum_{k=1}^N g_k c'_k = \sum_{k=1}^{N-1} (g_{k+1} - g_k - g_1) W_k + g_1 (q - \alpha c_1).$$

The proof of the above result is straightforward and consists of multiplying each equation by g_k , summing, and grouping like terms.

Theorem 4.3.3. *There exist a unique solution of the initial value problem on $[0, \infty)$ with $c_k(t) > 0$ for all $t > 0$ and $1 \leq k \leq N$.*

Proof: Local existence and uniqueness are obtained by a standard argument in ordinary differential equations theory.

Let $g_k = k$ in Lemma 4.3.2. Then

$$\sum_{k=1}^N k c'_k = q - \alpha c_1.$$

It follows that on any bounded time interval, c is bounded so there is a continuation

to $[0, \infty)$.

4.4 The equilibrium solution and its stability

We first show that the system (4.2.1) has a unique equilibrium solution.

Lemma 4.4.1. *The unique equilibrium of (4.2.1) is given by*

$$c_k = Q_k(q), \quad (4.4.1)$$

$$Q_1(q) = \frac{q}{\alpha}, \quad Q_k(q) = \frac{2q}{\alpha} (r(q))^{k-1} \text{ for } k \geq 2, \quad (4.4.2)$$

where

$$r(q) = \frac{\beta q}{\alpha f}. \quad (4.4.3)$$

Proof: We begin by showing that for an equilibrium c , $W_k(c) = 0$ for $1 \leq k \leq N$.

From the final equation $W_{N-1}(c) = 0$. For $2 \leq k \leq N - 1$, c satisfies

$$W_k(c) = W_{k-1}(c).$$

Since $W_{N-1}(c) = 0$ it follows that $W_k(c) = 0$ for $1 \leq k \leq N - 1$.

From the equation for c'_1 it follows that

$$c_1 = \frac{q}{\alpha}.$$

Since $W_1(c) = \beta c_1^2 - \frac{f}{2}c_2$ it follows that

$$c_2 = \frac{2\beta q^2}{f\alpha} = \frac{2qr(q)}{\alpha}.$$

For $k \geq 2$,

$$W_k(c) = \beta c_1 c_{k-1} - f c_k,$$

so iterating $W_k(c) = 0$ we obtain (4.4.2).

The quantity $r(q)$ in (4.4.3) is called the polymerization ratio and is an important parameter in the problem. In physical terms, r is equal to the product of the coagulation and production rates divided by the product of the fragmentation and loss rates. Another important physical parameter is the total amyloid-beta concentration in the brain, that is, the total number of amyloid-beta molecules. It is given by

$$\rho(t) = \sum_{k=1}^N k c_k. \tag{4.4.4}$$

From Lemma 4.4.1, at equilibrium this is equal to

$$\rho = \frac{q}{\alpha} + \frac{2q}{\alpha} \sum_{k=2}^N k r^{k-1}.$$

We can find an exact expression for ρ by considering

$$r^2 + r^3 + \dots + r^N = \frac{r^2 - r^{N+1}}{1 - r}$$

and differentiating to get a formula for

$$2r + 3r^2 + \dots + Nr^{N-1}.$$

The final result is

$$\rho = \frac{q}{\alpha} + \frac{2q}{\alpha} \left[\frac{2r - r^2 - (N+1)r^N + Nr^{N+1}}{(1-r)^2} \right]. \quad (4.4.5)$$

In our application we have that $0 < r < 1$. Hence for large N , the r^N and r^{N+1} terms are very small and a very good approximation for ρ is

$$\rho \approx \frac{q}{\alpha} \left(\frac{2}{(1-r)^2} - 1 \right).$$

To prove the stability of the equilibrium we will make use of the theory of Lyapunov function (see [23] Chapter 2). Consider the differential equation in \mathbf{R}^n ,

$$x' = g(x) \quad (4.4.6)$$

with an equilibrium $x = b$. Let \mathcal{G} be an open neighbourhood of b and let $V : \mathcal{G} \rightarrow \mathbf{R}$ be a continuously differentiable function. For a solution $x(t)$ of (4.4.6) we define the derivative of V by

$$V'(x) = \frac{d}{dt}V(x(t)).$$

Then V is a Lyapunov function on \mathcal{G} if the following two conditions hold:

- (i) $V(b) = 0$ and $V(x) > 0$ for $x \in \mathcal{G}$ with $x \neq b$.

(ii) $V'(x) \leq 0$ for all $x \in \mathcal{G}$.

The next result will enable us to prove global asymptotic stability.

Theorem 4.4.2. *Let $x = b$ be an equilibrium for (4.4.6) and V be a Lyapunov function on a neighbourhood \mathcal{G} of b with*

$$V'(x) < 0 \quad \text{for} \quad x \in \mathcal{G} \text{ with } x \neq b.$$

Then if $x(t)$ is a solution in \mathcal{G} , $x(t) \rightarrow b$ as $t \rightarrow \infty$.

We will make use of the function [2]

$$V(c) = \sum_{k=1}^N c_k \left(\ln \left(\frac{c_k}{Q_k} \right) - 1 \right) + \sum_{k=1}^N Q_k. \quad (4.4.7)$$

Using Lemma 4.3.2, a calculation shows that

$$\frac{dV(c)}{dt} = \sum_{k=1}^{N-1} \ln \left(\frac{c_{k+1} Q_k Q_1}{Q_{k+1} c_k c_1} \right) + \ln \left(\frac{c_1}{Q_1} \right) (q - \alpha c_1). \quad (4.4.8)$$

Theorem 4.4.3. *For any solution $c(t)$ of (4.2.1) with $c(0) \geq 0$ we have that for all k*

$$\lim_{t \rightarrow \infty} c_k(t) = Q_k.$$

Proof: If $c = (Q_k)$ then

$$V(c) = \sum_{k=1}^N \left[Q_k \left(\ln \left(\frac{Q_k}{Q_k} \right) - 1 \right) + Q_k \right] = 0.$$

For $m > 0$ and $x > 0$, the function $\theta(x) = x \left[\ln \left(\frac{x}{m} \right) - 1 \right]$ has an absolute minimiser

at $x = m$, so that $\theta(x) > -m$ if $x \neq m$. It follows that if c is not equal to the equilibrium then $V(c) > 0$.

In order to show that $V(c)$ is decreasing along solutions of (4.2.1), we use the inequality

$$(x - y)(\ln x - \ln y) \geq 0 \quad (4.4.9)$$

with equality if and only if $x = y$. This follows from the inequality

$$(z - 1) \ln z \geq 0$$

with equality if and only if $z = 1$.

To prove $V'(c) \leq 0$ with equality if and only if c is the equilibrium we show that each term in (4.4.8) is non-positive. For $2 \leq k \leq N - 1$,

$$\frac{Q_k Q_1}{Q_{k+1}} = \left(\frac{\alpha f}{\beta q} \right) \frac{q}{\alpha} = \frac{q}{\alpha r} = \frac{f}{\beta}.$$

Hence for $2 \leq k \leq N - 1$

$$\ln \left(\frac{c_{k+1} Q_k Q_1}{Q_{k+1} c_k c_1} \right) = \ln \left(\frac{c_{k+1} f}{\beta c_1 c_k} \right) (\beta c_1 c_k - f c_{k+1}).$$

From (4.4.9) it follows that the above term is non-positive and is equal to zero if and only if $W_k(c) = 0$.

Since

$$\frac{Q_1^2}{Q_2} = \frac{q^2 \alpha f}{\alpha^2 2q^2 \beta} = \frac{f}{2\beta},$$

the $k = 1$ term in (4.4.8) is

$$\ln \left(\frac{c_2 f}{2\beta c_1^2} \right) \left(\beta c_1^2 - \frac{f}{2} c_2 \right).$$

From (4.4.9) this is non-positive and is equal to zero if and only if $W_1(c) = 0$.

Finally,

$$\ln \left(\frac{c_1}{Q_1} \right) (q - \alpha c_1) = \ln \left(\frac{\alpha c_1}{q} \right) (q - \alpha c_1)$$

and this again is non-positive and is equal to zero if and only if $\alpha c_1 = q$.

The above calculations show that

$$\frac{dV}{dt} \leq 0$$

with equality if and only if c is the equilibrium.

The result follows from Theorem 4.4.2.

4.5 Effect of treatment

From Section 4.4, the approximation value of the total amyloid-beta concentration

($A\beta$ burden) at equilibrium is given by

$$\rho_\infty = \rho_\infty(q) = \frac{q}{\alpha} \left(\frac{2}{(1 - r(q))^2} - 1 \right),$$

where $r = r(q)$ is given by

$$r = \frac{\beta q}{\alpha f}.$$

The dynamics of the impact of a treatment can be assessed by changing the parameters. To lower the $A\beta$ burden we need to decrease r . One practical way to do this is reducing q by means of γ -secretase inhibitor.

To assess the impact of such a treatment we do the following numerics:

- (a) We first consider a symptomatic patient in the pre-treatment state. For this patient we assume that a steady state has been attained for the parameter values given in (4.2.3). Hence $c_k = Q_k(q)$ and the $A\beta$ burden is given approximately by $\rho_\infty(q)$. As in [8] we assume that this pre-treatment stay lasts for 250 days.
- (b) Continue the solution in (a) by solving the system with q replaced by $(0.6)q$. This represents treatment with the production rate q reduced by 40 %. We do this for a time period of approximately one year, say days 250-620. At day 620 the solution will be close to the equilibrium $c_k = Q_k((0.6)q)$. As we calculated in Section 4.4, this represents a 18-fold decrease in the $A\beta$ burden
- (c) At day 620 we remove the treatment. This means that we continue the solution from (b) using the original value q in system (4.2.1).

The results are shown in Figure 4.1.

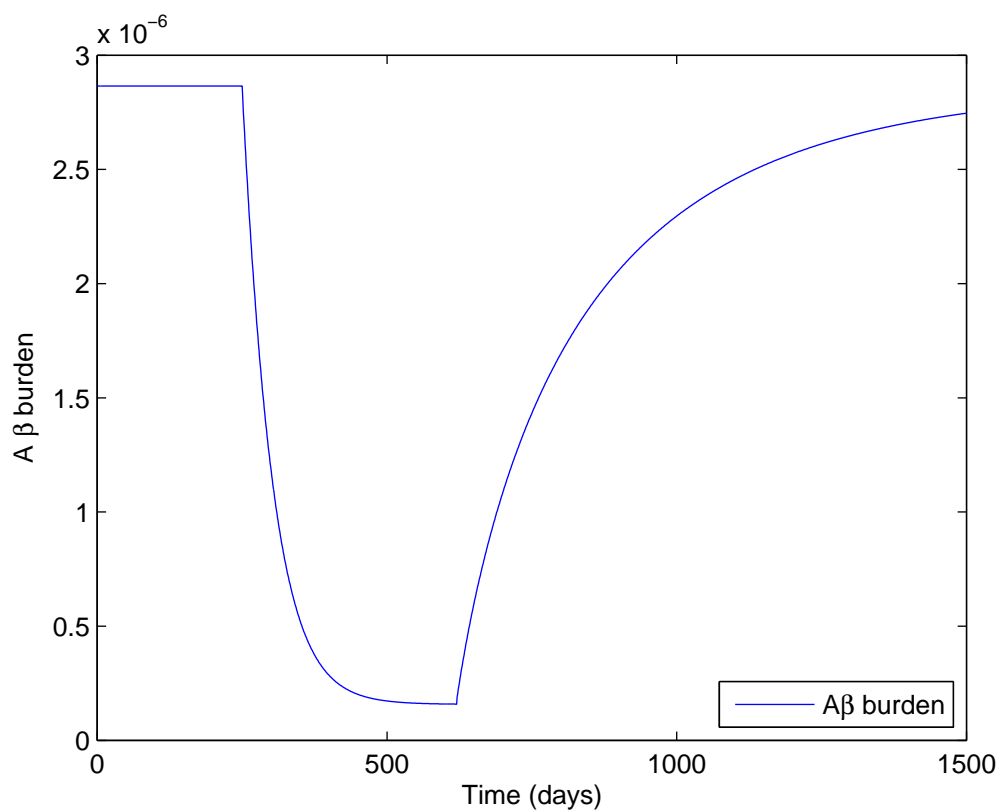


Figure 4.1: $A\beta$ burden for steps (a), (b) and (c).

In order to understand the long time periods involved in (b) and (c), we modify (b) and (c) into two mathematical problems.

Step B : The initial data for the system is calculated by using the equilibrium solution for the parameter values given by (4.2.3). Hence the initial data is

$$c_k(0) = Q_k(q). \quad (4.5.1)$$

To model the inhibitor reduction we replace q by $(0.6)q$ in (4.2.1) and solve with

initial data (4.5.1).

Step C : For this case the treatment is stopped. Hence we solve (4.2.1) with the parameter values (4.2.3) and the initial data

$$c_k(0) = Q_k((0.6)q). \quad (4.5.2)$$

Numerical solution for steps B and C are shown in Figure 4.2 and 4.3. Figure 4.2 is more or less the same as the portion of Figure 4.1 for days 250-620 with a similar statement for Figure 4.3. The point is that step B and step C are the same mathematical problem. We want to calculate the decay rate as a function of the parameters.

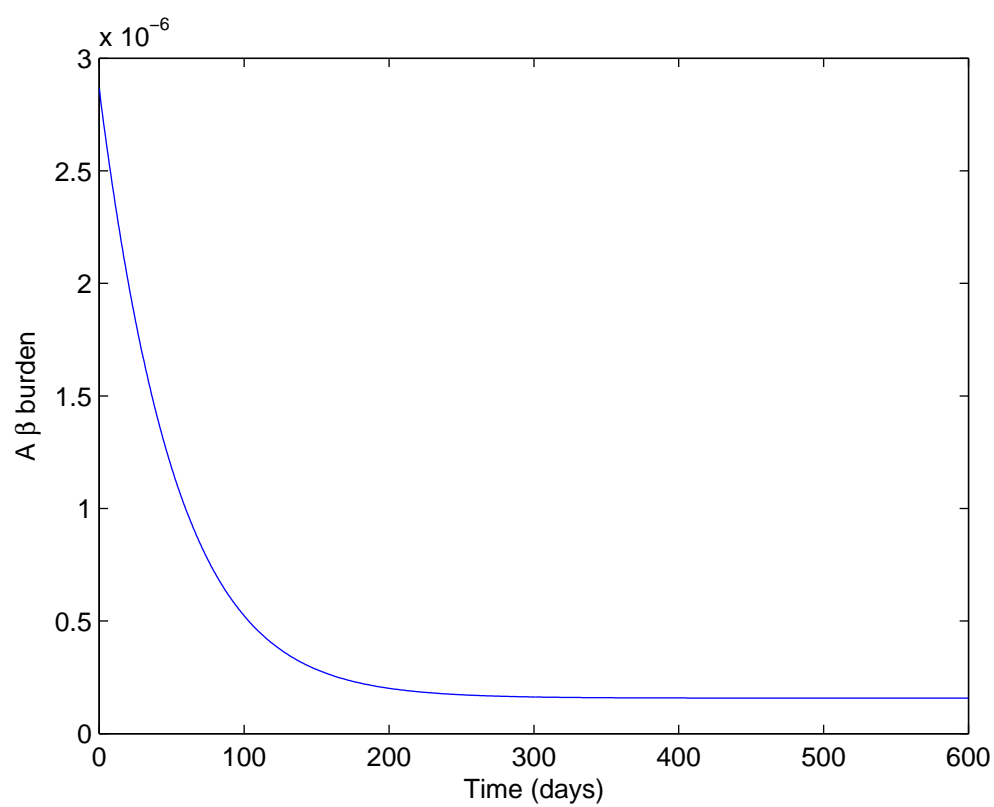


Figure 4.2: Step B calculation.

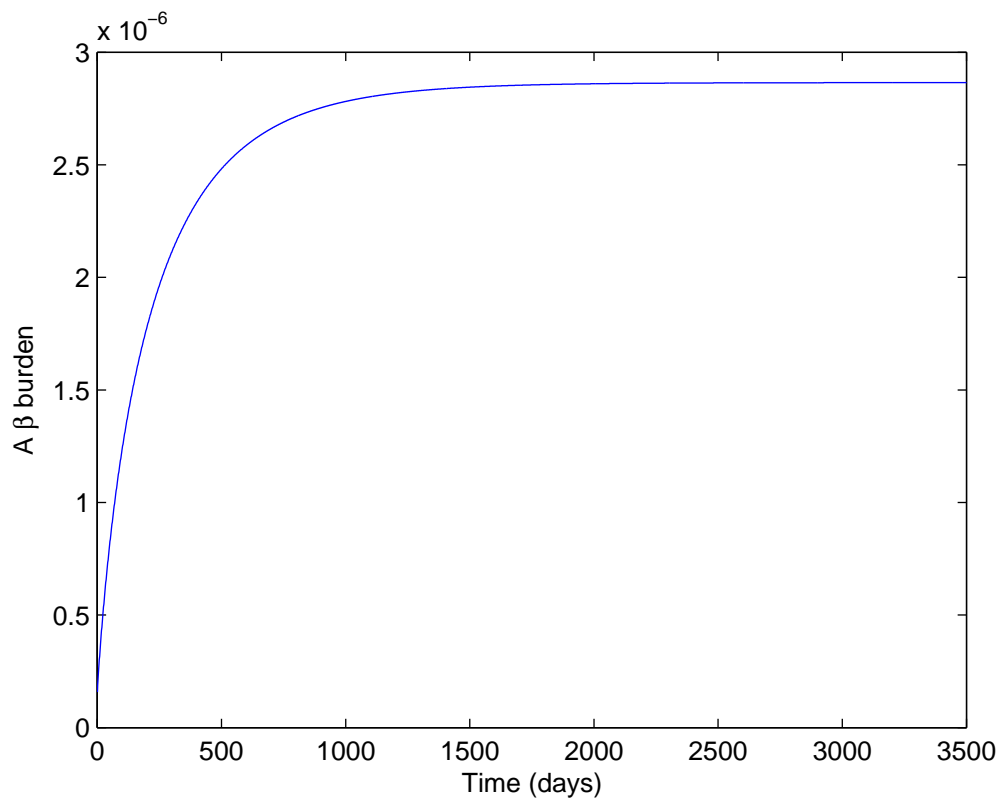


Figure 4.3: Step C calculation.

4.6 Estimate of the decay rate

In this section we develop an approximation to estimate the time scales involved in steps B and C from the previous section. For simplicity we describe step B.

For this case we replace q by $(0.6)q$ in (4.2.1). The equation for c_1 is

$$c_1' = (0.6)q - \alpha c_1 - W_1 - \sum_{k=1}^{N-1} W_k.$$

Numerical calculations show that c_1 decays to its equilibrium value $Q((0.6)q)$ very quickly. We show this in Figure 4.4. Hence to a very good approximation we can

replace $c_1(t)$ by its final constant value in (4.2.1)

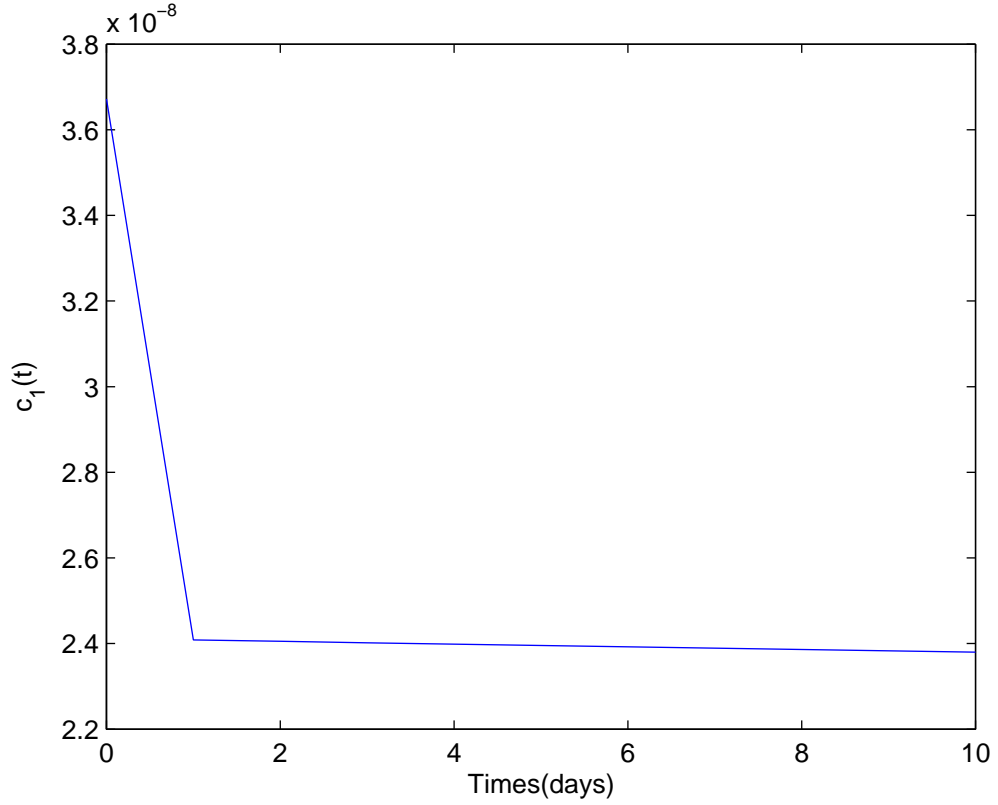


Figure 4.4: Rapid decay of $c_1(t)$ in step B.

The new set of equations are linear and are given by

$$\begin{aligned}
 c'_2 &= \beta z^2 - c_2 \left(\frac{f}{2} + \beta z \right) + f c_3 \\
 c'_k &= \beta z c_{k-1} - C_k (f + \beta z) + f c_{k+1}, \quad 3 \leq k \leq N-1 \\
 c'_N &= \beta z c_{N-1} - f c_N,
 \end{aligned} \tag{4.6.1}$$

where

$$z = Q_2((0.6)q) = \frac{(0.6)q}{\alpha}.$$

Equation (4.6.1) is of dimension $N - 1$ and the equilibrium $c_k = Q_k((0.6)q)$, $k = 2, 3, \dots, N$. We estimate the decay rate to this equilibrium. We make a change of variables to shift the equilibrium to the zero solution and to put the equation in symmetric form. Writing $Q_k = Q_k((0.6)q)$, let

$$c_k = Q_k + \sqrt{Q_k}x_k.$$

Then

$$\begin{aligned} \dot{x}_2 &= -\left(\frac{f}{2} + \beta z\right)x_2 + f\sqrt{\frac{Q_3}{Q_2}}x_3 \\ \dot{x}_k &= \beta z\sqrt{\frac{Q_{k-1}}{Q_k}}x_{k-1} - (f + \beta z)x_k + f\sqrt{\frac{Q_{k+1}}{Q_k}}x_{k+1}, \quad 3 \leq k \leq N-1 \\ \dot{x}_N &= \beta z\sqrt{\frac{Q_{N-1}}{Q_N}}x_{N-1} - fx_N. \end{aligned}$$

Define m by

$$m = f\sqrt{\frac{Q_{k+1}}{Q_k}}. \tag{4.6.2}$$

Since

$$f\sqrt{\frac{Q_{k+1}}{Q_k}} = \frac{fr}{r^{\frac{1}{2}}} = \frac{\beta z}{r^{\frac{1}{2}}}$$

it follows that

$$m = f\sqrt{\frac{Q_{k+1}}{Q_k}} = \beta z\sqrt{\frac{Q_{k-1}}{Q_k}}.$$

Writing $a = -f - \beta z$, the equations take the form

$$\frac{d\underline{x}}{dt} = A\underline{x} \quad (4.6.3)$$

where \underline{x} is the $(N - 1)$ vector $[x_2, x_3, \dots, x_N]^\perp$ and

$$A = \begin{bmatrix} a + f/2 & m & 0 & \cdots & 0 \\ m & a & m & & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & & m & a & m \\ 0 & \cdots & 0 & m & a + \beta z \end{bmatrix}.$$

Since A is symmetric, it has real eigenvalues and the decay rate will depend on its largest eigenvalue.

Define a new matrix B by

$$B = \frac{A - aI}{m} = \begin{bmatrix} f/2m & 1 & 0 & \cdots & 0 \\ 1 & 0 & 1 & & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & & 1 & 0 & 1 \\ 0 & \cdots & 0 & 1 & \beta z/m \end{bmatrix}.$$

If λ is an eigenvalue of A and μ is an eigenvalue of B then $\lambda = m\mu + a$. We order the eigenvalues of B as

$$\mu_1 \geq \mu_2 \geq \dots \geq \mu_{N-1}.$$

In fact we have strict separation in the above inequalities, that is

$$\mu_1 > \mu_2 > \dots > \mu_{N-1}.$$

This follows from the fact that the sub and super-diagonal entries of the tridiagonal matrix B are non zero. (See Section 37 in Chapter 5 of [45]).

The matrix B is a perturbation of the matrix C

where

$$C = \begin{bmatrix} 0 & 1 & 0 & \dots & 0 \\ 1 & 0 & 1 & & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & & 1 & 0 & 1 \\ 0 & \dots & 0 & 1 & 0 \end{bmatrix}.$$

The eigenvalues of C are known [46] and are given by

$$2 \cos \left(\frac{k\pi}{N} \right), \quad k = 1, \dots, N - 1.$$

There are many papers on the eigenvalues of tridigonal matrices which are perturbations of C , see for example [12]. We use the special structure of our matrix B to give a proof of the estimate of the eigenvalue μ . To obtain the estimates we use the Gerschgorin Circle Theorem and the Separation Theorem.

The following results are taken from (Section 13 in Chapter 2 of [45]). The matrix K with entries K_{ij} is a real matrix.

Theorem 4.6.1. Let C_i be the disk with centre k_{ij} and radius $\sum_{j=1, j \neq i}^n |k_{ij}|$ in the complex plane so that

$$C_i = \left\{ z \in \mathbb{C} : |z - k_{ii}| \leq \sum_{j=1, j \neq i}^n |k_{ij}| \right\}.$$

Then

- (a) The eigenvalues of A are contained in the union of the disks C_i .
- (b) If r of the disks do not intersect the remaining $n-r$, then the union of the r disks contain precisely k eigenvalues with $n-k$ eigenvalues in the other part.

Theorem 4.6.2. (Separation Theorem)

Suppose that K is a symmetric matrix with eigenvalues

$$\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n.$$

Let K' be a principle $(n-1) \times (n-1)$ submatrix with eigenvalues

$$\lambda'_1 \geq \lambda'_2 \geq \dots \geq \lambda'_{n-1}.$$

Then the following separation property holds

$$\lambda_s \geq \lambda'_s \geq \lambda_{s+1}, \quad \text{for } s = 1, 2, \dots, n-1.$$

Theorem 4.6.3. The largest eigenvalue μ_1 of B is bounded by

$$2 \cos \left(\frac{\pi}{N-2} \right) \leq \mu_1 \leq 2. \quad (4.6.4)$$

Proof We first prove the upper bounds. By the Gerschgorin Theorem, the maximum value of μ_1 is

$$\mu_1 \leq \max \left(2, 1 + \frac{f}{2m}, 1 + \frac{\beta z}{m} \right).$$

Since the $f/2m$ and $\beta z/m$ are < 1 , we have that $\mu_1 \leq 2$.

To prove the lower bound for μ_1 we apply the Separation Theorem twice. We first let $K = B$ and let K' be the $(N-2) \times (N-2)$ matrix obtained from K by deleting the last column and row. If the eigenvalues of K' are μ'_s then by the Separation Theorem

$$\mu_s \geq \mu'_s \geq \mu_{s+1}, \quad \text{for } s = 1, 2, \dots, N-2. \quad (4.6.5)$$

Now let K'' be the matrix obtained from K' by deleting the first column and row and let μ''_s be its eigenvalues. The $(N-3) \times (N-3)$ matrix K'' has zero diagonal and constant sub and super diagonal entries equal to 1 so that

$$\mu''_s = 2 \cos \left(\frac{s\pi}{N-2} \right), \quad \text{for } s = 1, 2, \dots, N-3.$$

By the Separation Theorem

$$\mu'_s \geq 2 \cos \left(\frac{s\pi}{N-2} \right) \geq \mu'_{s+1}, \quad \text{for } s = 1, 2, \dots, N-3. \quad (4.6.6)$$

Combining (4.6.5) and (4.6.6) we obtain

$$\mu_1 \geq 2 \cos \left(\frac{\pi}{N-2} \right)$$

and this completes the proof of the Theorem.

Using (4.6.4), the largest eigenvalues λ_1 of B is bounded by

$$a + 2m \cos\left(\frac{\pi}{N-2}\right) \leq \lambda_1 \leq a + 2m. \quad (4.6.7)$$

Since N is large, the cosine is very close to $\cos(0) = 1$ so that

$$\lambda_1 = a + 2m$$

is a very good approximation. Using this approximation

$$\lambda_1 = -(f + \beta z) + \frac{2\beta z}{r^{\frac{1}{2}}}.$$

After some algebra, this reduces to

$$\lambda_1 = -f(1 - \sqrt{r})^2 \quad (4.6.8)$$

Numerical calculations show that this is a good estimate of the decay rate.

We first study the step B calculation given in Section 4.6. We use the parameter values given by (4.2.3) except that q is replaced by $(0.6)q$. Figure 4.4 showed the rapid decay of $c_1(t)$. Figure 4.5 shows the numerics for the modified density

$$F(t) = \sum_{k=1}^N kc_k \quad (4.6.9)$$

for the nonlinear equation (4.2.1) and the linear equation (4.6.1). The initial data for

both equations

$$c_k(0) = Q_k(q) \quad , \quad 2 \leq k \leq N.$$

Figure 4.5 shows that the linear approximation is very good. By (4.6.8), the predicted decay rate is

$$\lambda_1 = 0.0285 \tag{4.6.10}$$

where we have used $(0, 6)q$ to calculate r in (4.4.3).

We can also estimate the decay rate calculating

$$G(t) = \frac{\ln |F(t) - F(\infty)|}{t + 1}$$

with $F(t)$ given by (4.6.9). We calculate $F(\infty)$ from

$$c_k(\infty) = Q_k((0.6)q).$$

From the numerical solution of the linear equation we obtain

$$G(600) = 0.02937$$

which is close to (4.6.10).

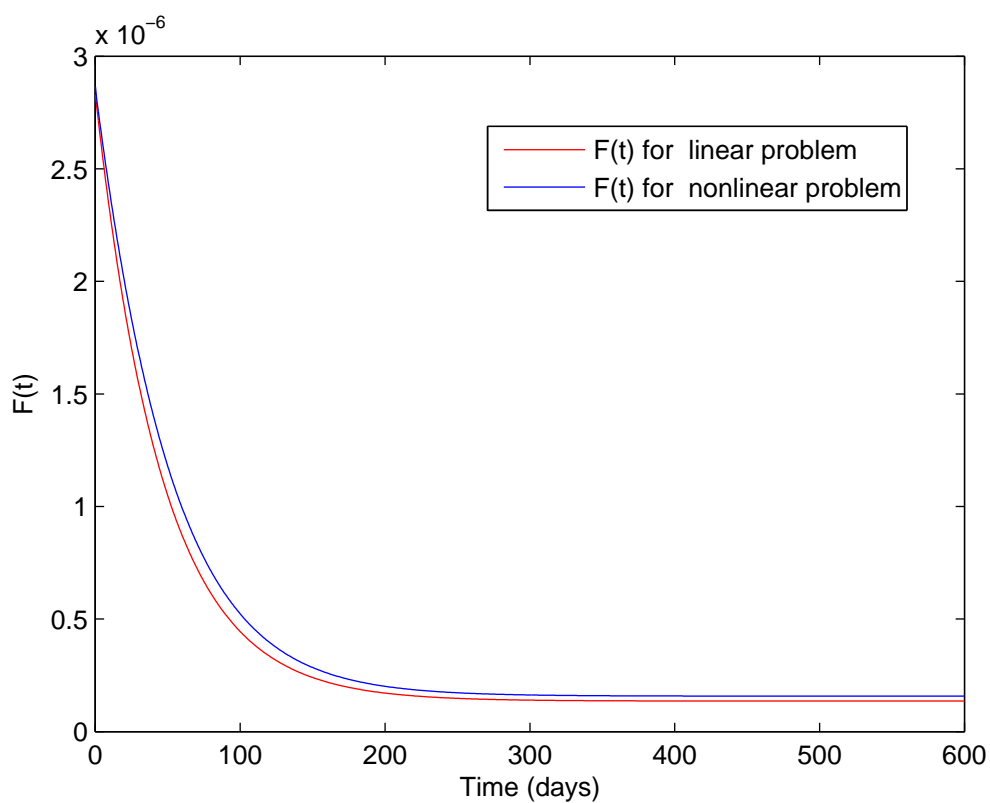


Figure 4.5: $F(t)$ for step B .

We can repeat the above for step C . Figure 4.6 shows the graph of $F(t)$ for the linear and nonlinear problem. Again the linear approximation is very good. From (4.6.8), the predicted decay rate for step C is

$$\lambda_1 = 0.0023. \tag{4.6.11}$$

where we have used q to calculate r in (4.4.3).

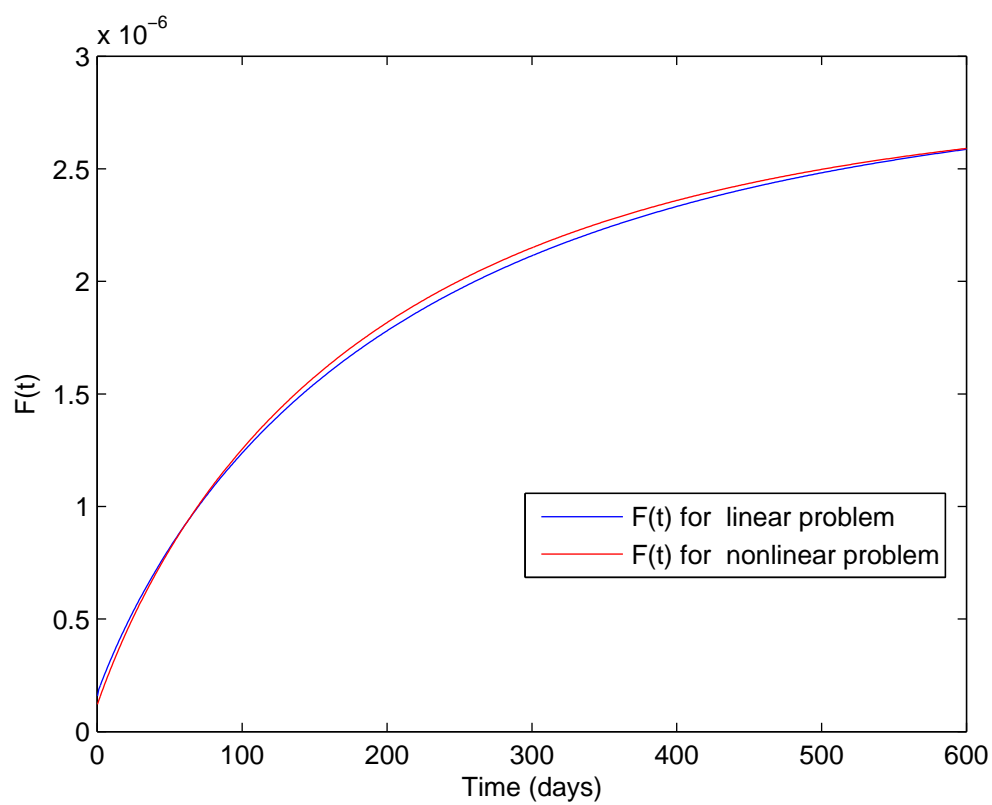


Figure 4.6: $F(t)$ for step C .

Chapter 5

Numerics of continuous coagulation - fragmentation

5.1 Continuous coagulation-fragmentation systems and the Smoluchowski equation

Continuous coagulation-fragmentation equations are types of partial integro-differential equations which are also known as aggregation-breakage equations. These models describe the dynamics of particle growth and the time evolution of a system of particles under the combined effect of coagulation and fragmentation. Each particle is identified by its size, which is assumed to be a positive real number and so is different from the discrete models discussed previously which have positive integer cluster sizes. From a physical point of view the basic mechanisms taken into account are the coalescence of two particles to form a larger one and the breakage of particles into smaller ones.

A continuous version of the coagulation-fragmentation equations is given by the

following integro differential equation [14, 42]:

$$\begin{aligned} \frac{\partial f(x, t)}{\partial t} &= \frac{1}{2} \int_0^x K(x-y, y) f(x-y, t) f(y, t) dy - \int_0^\infty K(x, y) f(x, t) f(y, t) dy \\ &\quad - \frac{1}{2} \int_0^x F(x-y, y) f(x, t) dy + \int_0^\infty F(x, y) f(x+y, t) dy, \end{aligned} \quad (5.1.1)$$

with

$$f(x, 0) = f_0(x) \geq 0.$$

Here f is the particle size distribution function and K , F are the coagulation and fragmentation kernels respectively determining the coagulation and fragmentation rates. They have the symmetry property $K(x, y) = K(y, x)$ and $F(x, y) = F(y, x)$.

The integrals on the right hand side of (5.1.1), which from left to right, represent:

- birth of particles of size x by the aggregation of particles with sizes y and $x-y$ ($0 \leq y \leq x$);
- death of particles of size x due to the aggregation with particles of size y ($0 \leq y < \infty$);
- death of particles of size x due to their breakage into particles of size y ($0 \leq y \leq x$);
- birth of particles of size x by the breakage of particles of size $x+y$ ($0 \leq y < \infty$).

Applications of these models can be found in many problems in chemistry, physics, astrophysics and meteorology, with specific examples in polymers, population balance, formation of stars, mergers of galaxies and atmospheric clouds [13, 15, 27].

We now focus on the coagulation process. The basic theory of particle coagulation was developed by Smoluchowski in 1917 [41] for the discrete particle size distribution. Smoluchowski proposed the following discrete model in order to apply the theory of Brownian motion to the coagulation of colloids which is known as the Smoluchowski coagulation equation:

$$\frac{dc_i}{dt} = \frac{1}{2} \sum_{j=1}^{i-1} K_{j,i-j} c_j c_{i-j} - \sum_{j=1}^{\infty} K_{i,j} c_i c_j$$

with

$$c_i(0) = c_i^0, \quad \text{for } i = 1, 2, 3, \dots$$

Here $c_i(t)$ is the number density of particles of size i at time t . The coagulation coefficients $K_{i,j}$ are non-negative real numbers such that $K_{i,j} = K_{j,i}$. The first term on the right-hand side of the above equation is the birth of particles of size i and the second is the death of particles of size i .

In 1928 Müller [34] provided the continuous version of the Smoluchowski equation:

$$\frac{\partial f(x, t)}{\partial t} = \frac{1}{2} \int_0^x K(x-y, y) f(x-y, t) f(y, t) dy - \int_0^{\infty} K(x, y) f(x, t) f(y, t) dy, \quad (5.1.2)$$

with

$$f(x, 0) = f_0(x).$$

Here the real variables $x \geq 0$ and $t \geq 0$ denote the size of the particles and time respectively. The number density of particles of size x at time t is denoted by $f(x, t)$. The coagulation coefficient is assumed to be symmetric so that $K(x, y) = K(y, x)$.

The only known closed exact solutions of (5.1.2) are for kernels

$$K(x, y) = 1, x + y \text{ and } xy. \quad (5.1.3)$$

Scott [37] used the Laplace transform and Wang [43] used similarity transformations to solve the coagulation equation (5.1.2) with kernels (5.1.3).

On the other hand, numerical solution methods have been derived and used for a wide range of kernels in many applications which we review briefly here.

In 1966 Friedlander and Wang [21, 44] used a similarity transform combined with numerical approximation for Brownian motion. In 1971 Cohn and Vaughan [7] approximated the coagulation equation by using a log-normal distribution in x for $f(x, t)$.

Krivitsky [27] obtained the numerical solution of the coagulation equation using a second-order Rung-Kutta method for kernels

$$K(x, u) = (x + y)^\lambda, (xy)^{\lambda/2}.$$

The solution with the kernel $(x + y)^\lambda$ where $0 < \lambda \leq 1$ and $(xy)^{\lambda/2}$ where $0 < \lambda \leq 2$ after some time becomes self-similar. The finite element technique [22] and the Spline-Galerkin method [16] have been used. The above methods have been used to obtain numerical results with the initial value

$$f(x, 0) = e^{-x}.$$

In the rest of this chapter we describe a piecewise constant in space approximation combined first with collocation in space and then in a full Galerkin approximation.

5.2 Piecewise constant collocation approximation

In this section we describe a piecewise constant in space approximation of the Smoluchowski equation. For numerical approximation the particle volume x should have a finite bound and we assume that for sufficiently large L , $u(x, t) = 0$ for $x > L$ and all t . The coagulation equation (5.1.2) is then approximated by

$$u_t = \frac{1}{2} \int_0^x K(y, x-y)u(y, t)u(x-y, t)dy - u(x, t) \int_0^L K(x, y)u(y, t)dy \quad (5.2.1)$$

for $0 \leq x \leq L$.

Suppose that $N + 1$ nodes are distributed on $[0, L]$ such that $0 = v_0 < v_1 < \dots < v_N = L$ and that the approximate solution $u_h(x, t) = u_{j+\frac{1}{2}}(t)$ when $x \in (v_j, v_{j+1})$. In all our examples we use uniform spaces points. Then setting $x = v_{k+1}$ and substituting u_h for u in (5.2.1), we have

$$\dot{u}_{k+\frac{1}{2}} = \frac{1}{2} \sum_{j=1}^{k+1} \int_{v_{j-1}}^{v_j} K(y, v_{k+1}-y)u_{j-\frac{1}{2}}u_{k-j+\frac{3}{2}}dy - u_{k+\frac{1}{2}} \sum_{j=1}^N \int_{v_{j-1}}^{v_j} K(v_{k+1}, y)u_{j-\frac{1}{2}}dy,$$

for $k = 0, \dots, N - 1$. We call this the piecewise constant space collocation scheme.

This approximation is directly related to the discrete coagulation equation (2.1.1) when we take $L, N \rightarrow \infty$ keeping $\frac{L}{N}$ fixed and make the following connections:

$$c_k = u_{k-\frac{1}{2}} \quad \text{for } k = 1, 2, \dots$$

and

$$a_{k,j} = \int_{v_{j-1}}^{v_j} k(v_k, y) dy.$$

We can then expect these approximations of the continuous problem to behave in the same ways as previously investigated for the discrete coagulation equation (2.1.1).

5.2.1 Numerical results

We test the above formulation of the approximation on the problem with initial value

$$u(x, 0) = e^{-x} \tag{5.2.2}$$

and the constant kernel $k(x, y) = 1$. The numerical results in Figure 5.2 and 5.3 indicate that the above scheme is first order, since the numerical error estimate

$$\epsilon_h(t) = \frac{L}{N} \sum_{j=1}^N v_{j-\frac{1}{2}} |u_{j-\frac{1}{2}}^N(t) - u_{3j-1-\frac{1}{2}}^{3N}(t)| \approx \int_0^L v |u^N(v, t) - u^{3N}(v, t)| dv \tag{5.2.3}$$

appears to be proportional to h . Here $u^N(v, t)$ is the approximate solution obtained with N mesh intervals of equal size and $u_{j-\frac{1}{2}}^N(t)$ is the value in the middle of the j th interval. Comparing $u_{j-\frac{1}{2}}^N$ with $u_{3j-1-\frac{1}{2}}^{3N}$ is a convenient way to estimate the error at the same space location. This weighted L_1 norm is related to the M_1 moment in the discrete problem, and measures the error in mass rather than number of particles. Similar results are obtained without the weight for the problems considered here. We have computed the approximation using $N = 20, 60, 180, 540, 1620, 4860, 14580$ with the space truncation parameter fixed at $L = 20$. In Figure 5.1 we compare the numerical results with the analytical solution for $k(x, y) = 1$ and initial value (5.2.2)

and the range of particles volume is truncated at $L = 100$ and $N = 1000$. This analytical solution to (5.1.2) for initial distribution (5.2.2) may be found in [37] and is given by

$$u(x, t) = \frac{4}{(t+2)^2} \exp\left(\frac{-2x}{t+2}\right). \quad (5.2.4)$$

Clearly from Figure 5.1 the truncation $L = 20$ ignores solution values of size $\leq 10^{-6}$, but these are relatively small compared to the errors for $v < L$.

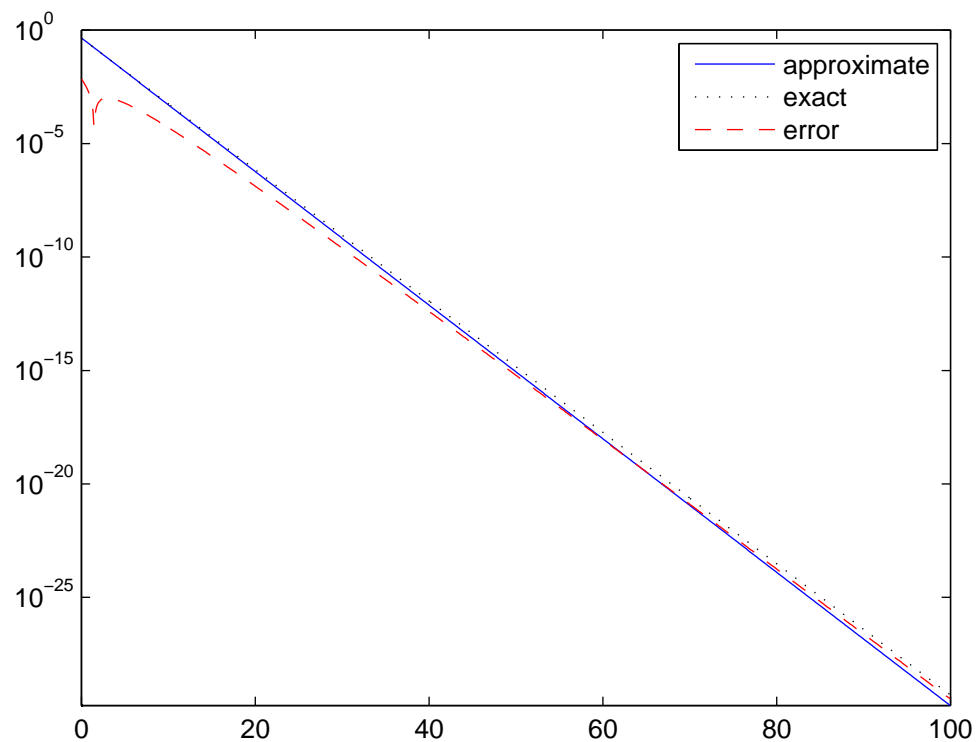


Figure 5.1: The comparison of the numerical piecewise approximation and analytical solution for the constant kernel $k(x, y) = 1$ with initial value (5.2.2) at $L = 100$, $N = 1000$ and $t = 1$.

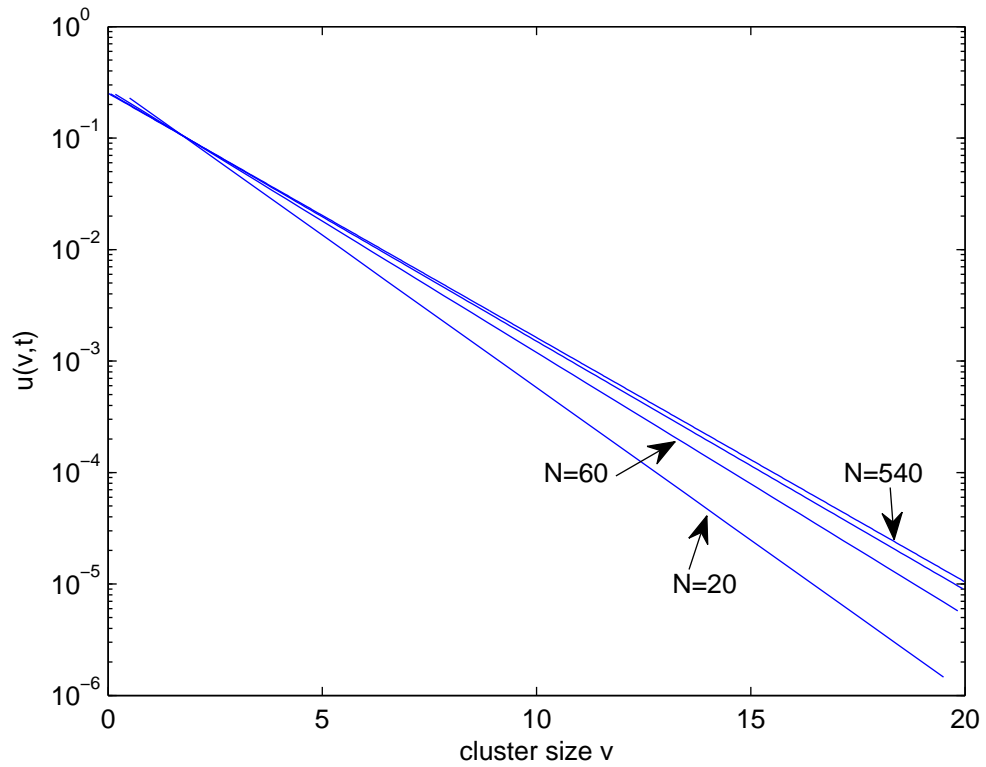


Figure 5.2: The convergence of the piecewise constant collocation approximation using $N = 20, 60, 180, 540$ and $L = 20$ for the constant kernel $k(x, y) = 1$ with initial value (5.2.2) at $t = 1$.

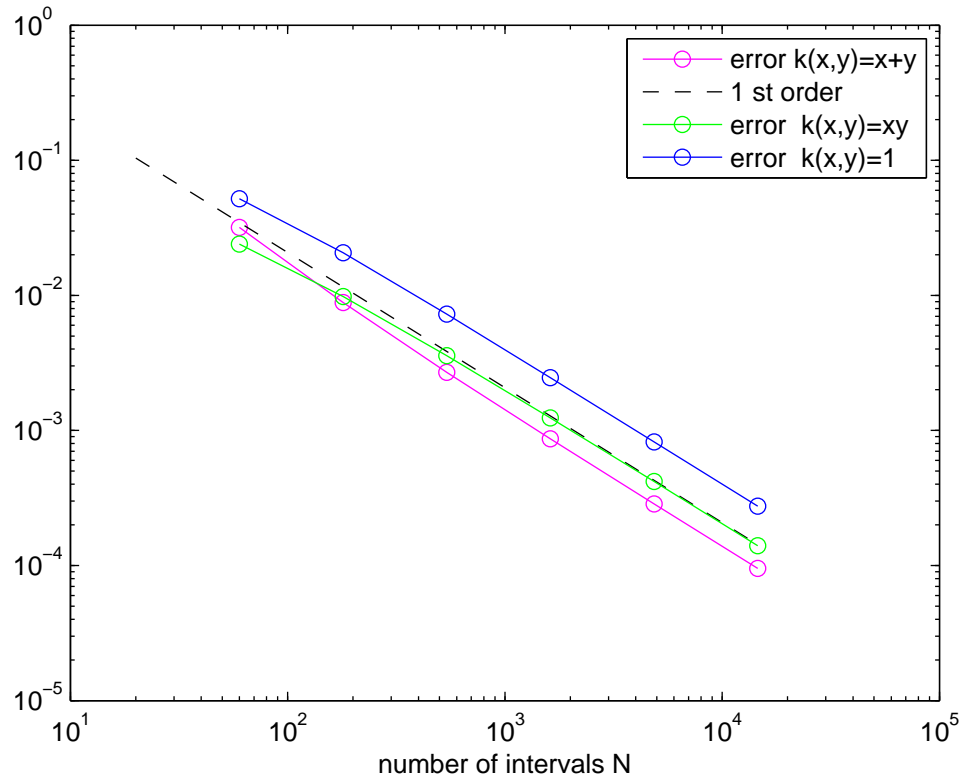


Figure 5.3: The numerical error ϵ_h defined by (5.2.3) using $N = 20, 60, 180, 540, 1620, 4860, 14580$ and $L = 20$ for the constant kernel $k(x, y) = 1, k(x, y) = x + y$ and $k(x, y) = xy$ with initial value (5.2.2) at $t = 1$. We see the error estimate appears to converge to 1st order.

5.3 Galerkin finite element approximation

Now we use the Galerkin FEM approximation to try to get more accurate results.

The approximate solution is represented in the same way as previously by

$$u_h = \sum_{j=0}^{N-1} u_{j+\frac{1}{2}}(t) \phi_{j+\frac{1}{2}}(x) \quad (5.3.1)$$

where we use piecewise constant basis functions

$$\phi_{k+\frac{1}{2}}(x) = \begin{cases} 1 & \text{when } x \in (v_k, v_{k+1}) \\ 0 & \text{otherwise.} \end{cases} \quad (5.3.2)$$

Also,

$$u_{h,t} = \frac{\partial}{\partial t} u_h = \sum_{j=0}^{N-1} \dot{u}_{j+\frac{1}{2}}(t) \phi_{j+\frac{1}{2}}(x). \quad (5.3.3)$$

However, the way to compute the $u_{j+1/2}(t)$ functions is different. We substitute u_h for u , multiply both sides of the equation (5.2.1) by $\phi_{k+\frac{1}{2}}(x)$ and integrate to get

$$\begin{aligned} \int_0^L u_{h,t} \phi_{k+\frac{1}{2}}(x) dx &= \frac{1}{2} \int_0^L \phi_{k+\frac{1}{2}}(x) \int_0^x k(y, x-y) u_h(y) u_h(x-y) dy dx \\ &\quad - \int_0^L \phi_{k+\frac{1}{2}}(x) u_h(x) \int_0^L k(x, y) u_h(y) dy dx. \end{aligned} \quad (5.3.4)$$

We write (5.3.4) as

$$F = D - C \quad (5.3.5)$$

where

$$F = \int_0^L u_{h,t} \phi_{k+\frac{1}{2}}(x) dx$$

$$D = \frac{1}{2} \int_0^L \phi_{k+\frac{1}{2}}(x) \int_0^x k(y, x-y) u_h(y) u_h(x-y) dy dx$$

and

$$C = \int_0^L \phi_{k+\frac{1}{2}}(x) u_h(x) \int_0^L k(x, y) u_h(y) dy dx,$$

and then examine each of these expressions in turn.

Using (5.3.1) , (5.3.2) and (5.3.3)

$$\begin{aligned}
 F &= \int_0^L u_{h,t} \phi_{k+\frac{1}{2}}(x) dx \\
 &= \int_{v_k}^{v_{k+1}} u_{h,t} dx \\
 &= \int_{v_k}^{v_{k+1}} \sum_{j=0}^{N-1} \dot{u}_{j+\frac{1}{2}} \phi_{j+\frac{1}{2}}(x) dx \\
 &= \int_{v_k}^{v_{k+1}} \dot{u}_{k+\frac{1}{2}} \phi_{k+\frac{1}{2}}(x) dx \\
 &= \Delta v \dot{u}_{k+\frac{1}{2}}, \tag{5.3.6}
 \end{aligned}$$

for $k = 0, \dots, N - 1$.

Next, using (5.3.1) and (5.3.2) we get that

$$\begin{aligned}
 D &= \frac{1}{2} \int_0^L \phi_{k+\frac{1}{2}}(x) \int_0^x k(y, x-y) u_h(y) u_h(x-y) dy dx \\
 &= \frac{1}{2} \int_{v_k}^{v_{k+1}} \int_0^x k(y, x-y) u_h(y) u_h(x-y) dy dx \\
 &= \frac{1}{2} \int_{v_k}^{v_{k+1}} \sum_{j=0}^k \int_{v_j}^{v_{j+1}} k(y, x-y) u_h(y) u_h(x-y) dy dx \\
 &= \frac{1}{2} \int_{v_k}^{v_{k+1}} \sum_{j=0}^k \int_{v_j}^{v_{j+1}} k(y, x-y) u_{j+\frac{1}{2}} \phi_{j+\frac{1}{2}} u_h(x-y) dy dx \\
 &= \frac{1}{2} \int_{v_k}^{v_{k+1}} \sum_{j=0}^k \int_{v_j}^{v_{j+1}} k(y, x-y) u_{j+\frac{1}{2}} u_h(x-y) dy dx. \tag{5.3.7}
 \end{aligned}$$

Now we need to expand (5.3.7), and get

$$\begin{aligned}
 D &= \frac{1}{2} \int_{v_k}^{v_{k+1}} \sum_{j=0}^{k-1} u_{j+\frac{1}{2}} \int_{v_j}^{v_{j+1}} k(y, x-y) u_h(x-y) dy dx \\
 &\quad + \frac{1}{2} \int_{v_k}^{v_{k+1}} u_{k+\frac{1}{2}} \int_{v_k}^x k(y, x-y) u_{\frac{1}{2}} dy dx.
 \end{aligned} \tag{5.3.8}$$

Now if we put $\mu = x - y$ then $y = x - \mu$ and $d\mu = -dy$ giving

$$\begin{aligned}
 I_j(x) &= u_{j+\frac{1}{2}} \int_{v_j}^{v_{j+1}} k(y, x-y) u_h(x-y) dy \\
 &= u_{j+\frac{1}{2}} \int_{x-v_{j+1}}^{x-v_j} k(x-\mu, \mu) u_h(\mu) d\mu. \\
 &= u_{j+\frac{1}{2}} \left[\int_{x-v_{j+1}}^{v_{k-j}} k(x-\mu, \mu) u_{k-j-\frac{1}{2}} d\mu + \int_{v_{k-j}}^{x-v_j} k(x-\mu, \mu) u_{k-j+\frac{1}{2}} d\mu \right] \\
 &= u_{j+\frac{1}{2}} u_{k-j-\frac{1}{2}} \int_{x-v_{j+1}}^{v_{k-j}} k(x-\mu, \mu) d\mu \\
 &\quad + u_{j+\frac{1}{2}} u_{k-j+\frac{1}{2}} \int_{v_{k-j}}^{x-v_j} k(x-\mu, \mu) d\mu.
 \end{aligned} \tag{5.3.9}$$

Using (5.3.8) and (5.3.9) we have

$$\begin{aligned}
 D &= \frac{1}{2} \int_{v_k}^{v_{k+1}} \sum_{j=0}^{k-1} I_j(x) dx + \frac{1}{2} u_{k+\frac{1}{2}} u_{\frac{1}{2}} \int_{v_k}^{v_{k+1}} \int_{v_k}^x k(y, x-y) dy dx \\
 &= \frac{1}{2} \int_{v_k}^{v_{k+1}} \sum_{j=0}^{k-1} u_{j+\frac{1}{2}} u_{k-j-\frac{1}{2}} \int_{x-v_{j+1}}^{v_{k-j}} k(x-\mu, \mu) d\mu \\
 &\quad + u_{j+\frac{1}{2}} u_{k-j+\frac{1}{2}} \int_{v_{k-j}}^{x-v_j} k(x-\mu, \mu) d\mu dx + \frac{1}{2} u_{k+\frac{1}{2}} u_{\frac{1}{2}} \int_{v_k}^{v_{k+1}} \int_{v_k}^x k(y, x-y) dy dx.
 \end{aligned}$$

We finally rewrite this as

$$\begin{aligned}
 D &= \frac{1}{2} \sum_{j=0}^{k-1} u_{j+\frac{1}{2}} u_{k-j-\frac{1}{2}} c_{jk} + \frac{1}{2} \sum_{j=0}^{k-1} u_{j+\frac{1}{2}} u_{k-j+\frac{1}{2}} d_{jk} + \frac{1}{2} u_{k+\frac{1}{2}} u_{\frac{1}{2}} d_{kk} \\
 &= \frac{1}{2} \sum_{j=0}^{k-1} u_{j+\frac{1}{2}} u_{k-j-\frac{1}{2}} c_{jk} + \frac{1}{2} \sum_{j=0}^k u_{j+\frac{1}{2}} u_{k-j+\frac{1}{2}} d_{jk}
 \end{aligned} \tag{5.3.10}$$

where

$$\begin{aligned}
 c_{jk} &= \int_{v_k}^{v_{k+1}} \int_{x-v_{j+1}}^{v_{k-j}} k(x-\mu, \mu) d\mu dx \quad 0 \leq j, k \leq N-1, \\
 d_{jk} &= \int_{v_k}^{v_{k+1}} \int_{v_{k-j}}^{x-v_j} k(x-\mu, \mu) d\mu dx \quad 0 \leq j, k \leq N-1.
 \end{aligned}$$

Now the second part of the right hand side of (5.3.4) is

$$C = \int_0^L \phi_{k+\frac{1}{2}}(x) u_h(x) \int_0^L k(x, y) u_h(y) dy dx,$$

and using (5.3.1) and (5.3.2) we obtain that

$$\begin{aligned}
 C &= \int_{v_k}^{v_{k+1}} u_{k+\frac{1}{2}} \int_0^L k(x, y) u_h(y) dy dx \\
 &= \int_{v_k}^{v_{k+1}} u_{k+\frac{1}{2}} \left(\sum_{j=0}^{N-1} \int_{v_j}^{v_{j+1}} k(x, y) u_{j+\frac{1}{2}} dy \right) dx \\
 &= u_{k+\frac{1}{2}} \sum_{j=0}^{N-1} u_{j+\frac{1}{2}} \int_{v_k}^{v_{k+1}} \int_{v_j}^{v_{j+1}} k(x, y) dy dx \\
 &= u_{k+\frac{1}{2}} \sum_{j=0}^{N-1} u_{j+\frac{1}{2}} e_{jk}
 \end{aligned} \tag{5.3.11}$$

where

$$e_{jk} = \int_{v_k}^{v_{k+1}} \int_{v_j}^{v_{j+1}} k(x, y) dy dx$$

for $0 \leq j, k \leq N - 1$.

Now we combine (5.3.6), (5.3.10) and (5.3.11) in (5.3.5) to get

$$\begin{aligned} \Delta v \dot{u}_{k+\frac{1}{2}} &= \frac{1}{2} \sum_{j=0}^{k-1} u_{j+\frac{1}{2}} u_{k-j-\frac{1}{2}} c_{jk} + \frac{1}{2} \sum_{j=0}^k u_{j+\frac{1}{2}} u_{k-j+\frac{1}{2}} d_{jk} \\ &\quad - u_{k+\frac{1}{2}} \sum_{j=0}^{N-1} u_{j+\frac{1}{2}} e_{jk} \end{aligned} \quad (5.3.12)$$

for $0 \leq j, k \leq N - 1$

where

$$\begin{aligned} c_{jk} &= \int_{v_k}^{v_{k+1}} \int_{x-v_{j+1}}^{v_{k-j}} k(x - \mu, \mu) d\mu dx \\ d_{jk} &= \int_{v_k}^{v_{k+1}} \int_{v_{k-j}}^{x-v_j} k(x - \mu, \mu) d\mu dx \\ e_{jk} &= \int_{v_k}^{v_{k+1}} \int_{v_j}^{v_{j+1}} k(x, y) dy dx. \end{aligned}$$

5.3.1 Numerical results

Here we will consider the constant kernel $k(x, y) = 1$. In Figure 5.4 we compare the numerical results with the analytical solution for $k(x, y) = 1$ and initial value (5.2.2).

The range of particle size is truncated at $L = 100$ and $N = 1000$ equally spaced nodes are used. The numerical result in Figure 5.5 shows that the above scheme is second order, since the numerical error ϵ_h appears to be proportional to h^2 . We have computed the approximation using a number of points $N = 20, 60, 180, 540, 1620, 4860, 14580$ with the truncation parameter fixed at $L = 20$.

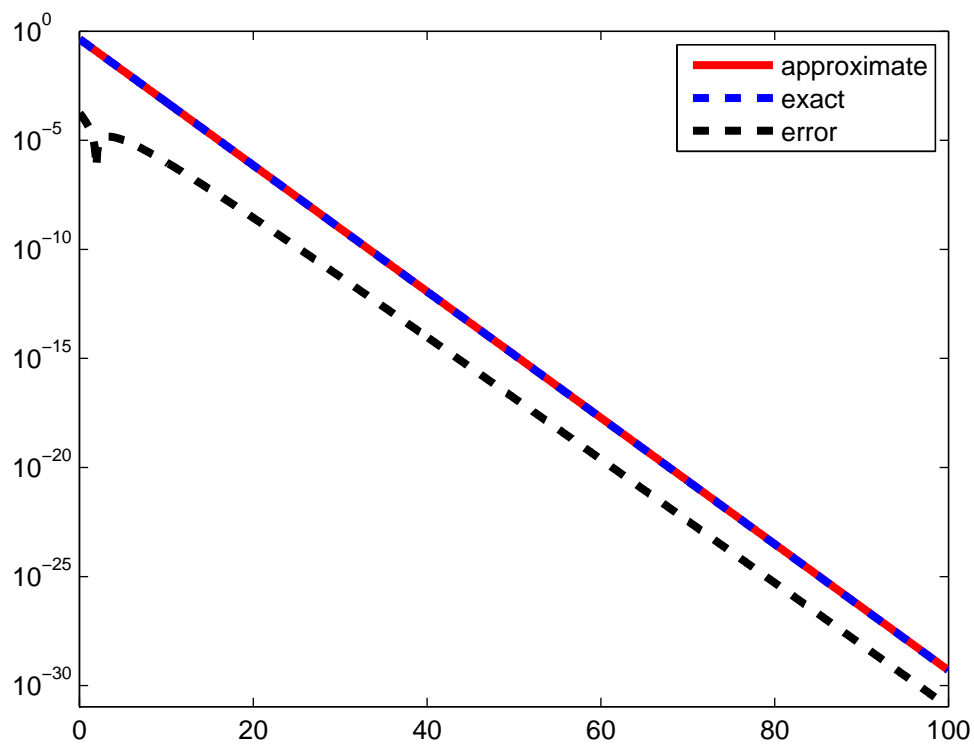


Figure 5.4: The comparison of the numerical Galerkin approximation and analytical solution for the constant kernel $k(x, y) = 1$ with initial value (5.2.2) at $L = 100$, $N = 1000$ and $t = 1$.

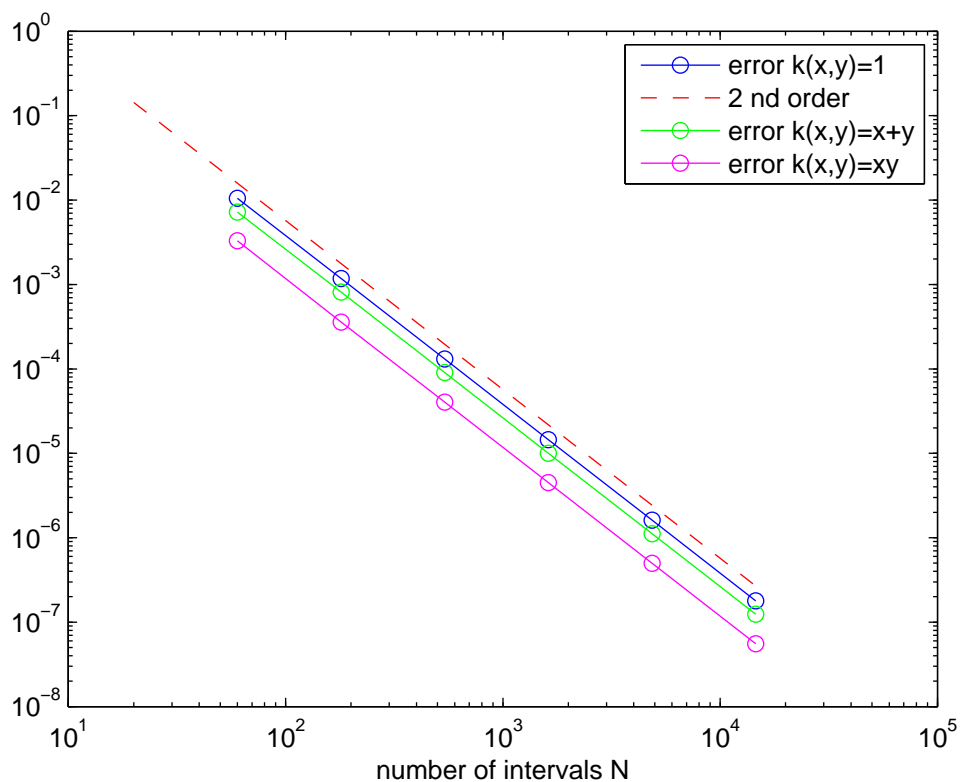


Figure 5.5: Computing the numerical error ϵ_h defined in (5.2.3) using $N = 20, 60, 180, 540, 1620, 4860, 14580$ and $L = 20$ for the constant kernel $k(x, y) = 1, k(x, y) = x + y$ and $k(x, y) = xy$ with initial value (5.2.2) at $t = 1$. We see the error estimates appear to be 2nd order.

Chapter 6

Concluding remarks

We have studied a number of topics in coagulation-fragmentation dynamics. These equations describe the evolution of clusters of particles which can coagulate to form larger particles or fragment to form smaller ones. An important issue is whether or not the density remains constant in time. Certain coagulation and fragmentation rates lead to the decrease of the density in finite time. This loss of mass is called gelation. In Chapter 2 we use formal calculations to investigate gelation in a number of examples. The one-parameter family of model in Example 2 in Section 2.2 is new.

Gelation only occurs in infinite-dimensional models of coagulation-fragmentation. Numerical methods are usually based on finite-dimensional approximations to these equations. It is important in developing numerical methods, to allow for the detection of gelation. To do this we use the approximation (2.3.7) in which density decreases and all solutions converge to zero as $t \rightarrow \infty$. Gelation events correspond to the formation of large clusters and are detected in (2.3.7) by a rapid decrease in density for some finite time. We use the approximation (2.3.7) in Chapter 2 to show that the method is well suited to the detection of gelation.

The only mathematical study of the finite-dimensional system (2.3.7) is for a very special case of pure coagulation. Chapter 3 contains a study of the decay rate of solutions to this equation. Assuming that the detailed balance condition holds, we obtain a very general result for coagulation-fragmentation equations. For a system of size n , the solution decays at a rate of order $t^{-1/n}$. This is very slow for large n . For the pure coagulation equation, we obtain various decay rate results in a number of special cases. Our results show that there is unlikely to be a general theory of decay rates for the pure coagulation case.

In Chapter 4 we study a model for the treatment of Alzheimer's disease. The model is a modified form of a special case of the coagulation fragmentation equations. We give a complete mathematical analysis of these equations. One important result is an approximation in terms of the parameters of the model for the time scales involved.

Chapter 5 we consider numerical approximations to the continuous version of the coagulation equations. These approximations are themselves discrete coagulation equations. We first consider a piecewise constant collocation in space approximation. We numerically solve the equation for the three coagulation coefficients,

$$K(x, y) = 1, x + y \text{ and } xy$$

for which exact solutions are available and show that it gives first order accurate results. We then use the Galerkin finite element approximation which gives second order accuracy convergence in tests.

Future work should include trying to relate results on the behaviour of the discrete problem to the behaviour of the numerical approximation of the continuous problem.

Also, the Galerkin approximation should be used to study the higher moments and future analysis for convergence carried out.

The results in Chapter 3 give a firm foundation for the study of the finite dimensional equation (2.3.7). However, much remains to be done. In particular it remains to give any mathematical results for the detection of gelation. A starting point could be the analysis of (2.3.7) for large n for some simple cases when there is gelation in the infinite problem.

Bibliography

- [1] J. M. Ball and J. Carr. The discrete coagulation-fragmentation equations: existence, uniqueness, and density conservation. *J. Statist. Phys.*, 61(1-2):203–234, 1990.
- [2] J. M. Ball, J. Carr, and O. Penrose. The Becker-Döring cluster equations: basic properties and asymptotic behaviour of solutions. *Comm. Math. Phys.*, 104(4):657–692, 1986.
- [3] J. P. Bourgade and F. Filbet. Convergence of a finite volume scheme for coagulation-fragmentation equations. *Math. Comp.*, 77(262):851–882, 2008.
- [4] J. Carr. *Applications of centre manifold theory*, volume 35 of *Applied Mathematical Sciences*. Springer-Verlag, New York-Berlin, 1981.
- [5] J. Carr. Asymptotic behaviour of solutions to the coagulation-fragmentation equations. I. The strong fragmentation case. *Proc. Roy. Soc. Edinburgh Sect. A*, 121(3-4):231–244, 1992.
- [6] J. Carr and F. P. da Costa. Instantaneous gelation in coagulation dynamics. *Z. Angew. Math. Phys.*, 43(6):974–983, 1992.

BIBLIOGRAPHY

- [7] E. R. Cohen and E.U. Vaughan. Approximate solution of the equations for aerosol agglomeration. *Journal of Colloid and Interface Science*, 35(4):612–623, 1971.
- [8] D. L. Craft, L. M. Wein, and D. J. Selkoe. *A Mathematical Model of the Impact of Novel Treatments on the $A\beta$ Burden in the Alzheimer's brain, CSF and Plasma*. 2002.
- [9] D. L. Craft, L. M. Wein, and D. J. Selkoe. The impact of novel treatment on $A\beta$ burden in the alzheimer's disease: insight from a mathematical model . *Operation Research and Health Care volume 70 of International Series in Operation Research and Management Science* , Kluwer Academic publishers., 2005.
- [10] F. P. da Costa. Existence and uniqueness of density conserving solutions to the coagulation-fragmentation equations with strong fragmentation. *J. Math. Anal. Appl.*, 192(3):892–914, 1995.
- [11] F. P. da Costa. A finite-dimensional dynamical model for gelation in coagulation processes. *J. Nonlinear Sci.*, 8(6):619–653, 1998.
- [12] C. M. da Fonseca. On the location of the eigenvalues of Jacobi matrices. *Appl. Math. Lett.*, 19(11):1168–1174, 2006.
- [13] R. L. Drake. A general mathematical survey of the coagulation equation. *In Topics in current aerosol research, part 2*, 203–376, 1972.
- [14] P. B. Dubovskii and I. W. Stewart. Existence, uniqueness and mass conservation for the coagulation-fragmentation equation. *Math. Methods Appl. Sci.*, 19(7):571–591, 1996.

BIBLIOGRAPHY

- [15] Pavel B. Dubovskii. *Mathematical theory of coagulation*, volume 23 of *Lecture Notes Series*. Seoul National University, Research Institute of Mathematics, Global Analysis Research Center, Seoul, 1994.
- [16] L. D. Erasmus, D. Eyre, and R. C. Everson. Numerical treatment of the population balance equation using a spline-galerkin method. *Computers Chem. Eng.*, 18(9):775–783, 1994.
- [17] M. H. Ernst, E. M. Hendriks, and R. M. Ziff. Exact solutions to the coagulation equation. *Phys. Lett. A*, 92(6):267–270, 1982.
- [18] M. Escobedo, Ph. Laurençot, S. Mischler, and B. Perthame. Gelation and mass conservation in coagulation-fragmentation models. *J. Differential Equations*, 195(1):143–174, 2003.
- [19] M. Escobedo, S. Mischler, and B. Perthame. Gelation in coagulation and fragmentation models. *Comm. Math. Phys.*, 231(1):157–188, 2002.
- [20] S. K. Friedlander. On the particle size spectrum of a condensing vapor. *Phys. Fluids*, 3:693–696, 1960.
- [21] S. K. Friedlander and C. S. Wang. The self-preserving particle size distribution for coagulation by brownian motion. *Journal of Colloid and Interface Science*, 22:126–132, 1966.
- [22] F. Gelbard and J. H. Seinfeld. Numerical solution of the dynamic equation for particulate system. *J. Comp. Phys.*, 28:375–375, 1978.

BIBLIOGRAPHY

- [23] Paul Glendinning. *Stability, instability and chaos: an introduction to the theory of nonlinear differential equations*. Cambridge Texts in Applied Mathematics. Cambridge University Press, Cambridge, 1994.
- [24] E. M. Hendriks, M. H. Ernst, and R. M. Ziff. Coagulation equations with gelation. *J. Statist. Phys.*, 31(3):519–563, 1983.
- [25] Intae Jeon. Existence of gelling solutions for coagulation-fragmentation equations. *Comm. Math. Phys.*, 194(3):541–567, 1998.
- [26] L. B. W. Jolley. *Summation of series*. 2nd revised ed. Dover Books on Advanced Mathematics. Dover Publications, Inc., New York, 1961.
- [27] D. S. Krivitsky. Numerical solution of the Smoluchowski kinetic equation and asymptotics of the distribution function. *J. Phys. A*, 28(7):2025–2039, 1995.
- [28] Wilson Lamb, Adam McBride, and Louise Smith. Coagulation and fragmentation processes with evolving size and shape profiles: a semigroup approach. *Discrete Contin. Dyn. Syst.*, 33(11-12):5177–5187, 2013.
- [29] F. Leyvraz. Existence and properties of post-gel solutions for the kinetic equations of coagulation. *J. Phys. A*, 16(12):2861–2873, 1983.
- [30] F. Leyvraz. Large time behaviour of the smoluchowski equations of coagulation. *Physical Review A*, 29(2):854, 1984.
- [31] F. Leyvraz. New exactly solvable models of Smoluchowski’s equations of coagulation. *J. Phys. A*, 18(2):321–326, 1985.

BIBLIOGRAPHY

- [32] F. Leyvraz and H. R. Tschudi. Singularities in the kinetics of coagulation processes. *J. Phys. A*, 14(12):3389–3405, 1981.
- [33] J. B. McLeod. On an infinite set of non-linear differential equations. *Quart. J. Math. Oxford Ser. (2)*, 13:119–128, 1962.
- [34] Müller. Zur allgemeinen theorie der raschen koagulation. *Kolloidchemische Beihefte*, 27:223–250, 1928.
- [35] O. Penrose and J. Lebowitz. Towards a rigorous theory of metastability. in: Studies in statistical mechanics,. *Vol. VII. Fluctuation phenomena. Montroll, E.W., Lebowitz, J.L. (eds).*, Amsterdam : North-Holland 1979.
- [36] O. Penrose, J. Lebowitz, J. Marro, M. Kalos, and J. Tobochnik. Kinetics of a first-order phase transition: computer simulations and theory. *J. Statist. Phys.*, 34(3-4):399–426, 1984.
- [37] W. T. Scott. Analytic studies of cloud droplet coalescence. *J. Atoms. Sci.*, 25:54–65, 1968.
- [38] D. J. Selkoe. Aging, amyloid, and alzheimer’s disease: A perspective in honor of carl cotman. *Neurochemical Research*, vol28,1705-1713,2003.
- [39] J. Silk and S. D. White. The development of structure in the expanding universe,. *Astrophysical Journal*,, 223:53–62, 1978.
- [40] M. Slemrod. A note on the kinetic equations of coagulation. *J. Integral Equations Appl.*, 3(1):167–173, 1991.

BIBLIOGRAPHY

- [41] M. V. Smoluchowski. Versuch einer mathematischen theorie der koagulation skinetic kolloider lösunger. *Z. Phys. Chem*, 92:129–168, 1917.
- [42] I. W. Stewart. A global existence theorem for the general coagulation-fragmentation equation with unbounded kernels. *Math. Methods Appl. Sci.*, 11(5):627–648, 1989.
- [43] C. S. Wang. A mathematical study of the particle size distribution of coagulating disperse system. *Ph.D. Thesis*, University of California, 1966.
- [44] C. S. Wang and S. K. Friedlander. The self-preserving particle size distribution for coagulation by brownian motion. *Journal of Colloid and Interface Science*, 24:170–179, 1967.
- [45] J. H. Wilkinson. *The algebraic eigenvalue problem*. Monographs on Numerical Analysis. The Clarendon Press, Oxford University Press, New York, 1988. Oxford Science Publications.
- [46] Wen-Chuan Yueh. Eigenvalues of several tridiagonal matrices. *Applied Mathematics E-notes*, 66-74,2005.