University of Alberta

THE DISCRETE COAGULATION-FRAGMENTATION MODEL WITH BILINEAR COAGULATION KERNEL AND CONSTANT FRAGMENTATION KERNEL

by

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ABSTRACT

Coagulation is the coalescence or aggregation of one or more small particles, or clusters of particles, to form larger clusters. The reverse procedure, which involves the break-up of large particles into smaller ones, is called fragmentation.

This thesis investigates the coagulation-fragmentation model. This model is described by an infinite set of nonlinear ODEs which can be transformed into a nonlinear PDE by means of a generating function. Our goal is to determine formulas for the number of size k clusters at time, t, and the total number of clusters at t. This requires deriving and solving the appropriate PDE. We will also discuss the total mass of the system which is needed to solve this PDE.

As well, we investigate a phenomenon known as gelation. Gelation is the break-down of conservation of mass. Specifically, our focus will be on whether the addition of fragmentation to a coagulation model delays gelation.

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Chapter 1

Introduction

Coagulation is the formation of larger clusters from smaller clusters. The rate at which this occurs is described by the coagulation kernel, $K_{j,k}$, where $j, k \in \mathbb{N}$ are the size of the clusters. A cluster of size k means it is a polymer made up of k particles (known as a monomer). Fragmentation is the reverse process (i.e. large clusters breaking apart to form smaller clusters). The rate at which this occurs is described by the fragmentation kernel, $L_{j,k}$. As well, we assume binary collisions between clusters. This means that at one time a cluster coalesces with another cluster only or fragments into exactly two smaller pieces. The simplest coagulation and fragmentation processes are illustrated in Figures 1.1a and 1.1b, respectively.

Because of the simplicity of this model, it has applications ranging from medical sciences, botany and chemistry to astrophysics and meteorology [7, 2, 4, 14].

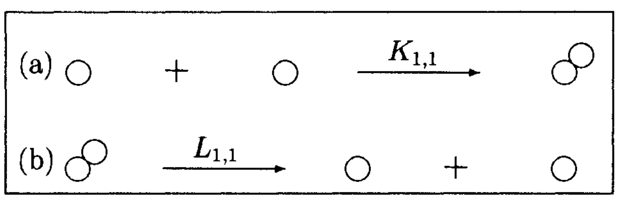

Figure 1.1: Elementary coagulation and fragmentation models.

In these fields, coagulation and fragmentation processes are conveniently used to model colloidal systems. For example, the coagulation-fragmentation model can describe the simultaneous polymerization-depolymerization of long chains of monomers [4]. In hematology, the coagulation model has been used to describe the formation of rouleaux, which are clusters of red blood cells resembling stacks of coins [14].

This area of research began in 1916 when Smoluchowski [23, 24] introduced his coagulation equation,

$$\frac{dN_k(t)}{dt} = \frac{1}{2}\sum_{j=1}^{k-1} K_{j,k-j}N_jN_{k-j} - \sum_{j=1}^{\infty} K_{j,k}N_jN_k. \tag{1.1}$$

Equation (1.1) represents the rate of change in the number of size k clusters per unit volume, $N_k(t)$, that are coalescing at time, $t \geq 0$. A detailed explanation will be provided in Chapter 2. Smoluchowski determined a solution for (1.1) under a constant coagulation kernel with monodisperse initial condition. Monodisperse initial condition means, at time zero, there is only one cluster of size one present, no other clusters exist.

Of popular interest is the coagulation model with product kernel, $K_{j,k} = jk$, because a paradoxical phenomenon known as gelation occurs. Gelation is the break down of conservation of mass in the system and is physically interpreted as the creation of an infinite size cluster (called a superparticle or gel). Its definition suggests that gelation maybe physically invalid. However consider, for example, the formation of a hail ball which represents the creation of a superparticle. Part of the mass of the system (i.e. the water droplets in the cloud) is transported to this superparticle (i.e. the hail ball); that is, gelation occurs. After gelation, the gel coexists with the remaining system. Towards this Ziff and Stell [26] proved the existence of post-gelation solutions. McLeod [11] proved without the occurrence of gelation, no solution exists for all time. Naturally, a couple of questions arise: what is the pre-gelation behaviour as opposed to the post-gelation behaviour and when is the gelation time (the time at which constant mass first fails)? A thorough explanation of these questions can be found in [25, 19, 8, 15, 16, 22].

Other coagulation kernels have also been investigated because it may be desirable to control the production of $N_k(t)$ by adjusting the coagulation kernel. The coagulation model with kernels $K_{j,k} = j + k$ and $K_{j,k} = A + B(j + k)$ have been studied in [19, 3, 15] where A and B are positive real numbers. The bilinear coagulation kernel, $K_{j,k} = A + B(j + k) + Cjk$, where $C \in \mathbb{R}_{\geq 0}$, has been studied in [16].

The coagulation-fragmentation model,

$$\frac{dN_k(t)}{dt} = \frac{1}{2}\sum_{j=1}^{k-1} K_{j,k-j}N_jN_{k-j} - \sum_{j=1}^{\infty} K_{j,k}N_jN_k + \sum_{j=1}^{\infty} L_{j,k}N_{j+k} - \frac{1}{2}\sum_{j=1}^{k-1} L_{j,k-j}N_k, \tag{1.2}$$

is investigated in this thesis. Equation (1.2) represents the rate of change in the number density of k size clusters at time, t, due to both coalescence and fragmentation. The first introduction of fragmentation to the coagulation model appears in Blatz and Tobolosky's 1944 paper [4]. They determined a particular solution for the constant coagulation and fragmentation kernels. Some time later, for the same kernels, Barrow determined an implicit solution to $N_k(t)$ in the continuous case of (1.2). Nonetheless, literature about (1.2) is sparse especially in comparison to its coagulation counterpart because the addition of fragmentation greatly complicates the model. Most of the literature focuses on existence and uniqueness solutions [12, 21, 20, 18, 6] with very few discussing explicit solutions for (1.2). This shortcoming motivates part of the work in this thesis.

A recent highlight of the coagulation-fragmentation model is the investigation of gelation. It is logical to assume with the addition of fragmentation that gelation time will increase because fragmentation counteracts the effect of coagulation therefore delaying the formation of a superparticle which characterizes gelation. Furthermore, da Costa [6] proved that, for sufficiently strong fragmentation, gelation is suppressed. But what defines 'strong' fragmentation? This is partially answered in Escobedo et al. [10, 9] for the continuous analogue of (1.2). They proved for $0 \leq \alpha \leq \beta \leq 1, \gamma \in \mathbb{R}$ and

$$K_{j,k} = j^\alpha k^\beta + j^\beta k^\alpha, \qquad L_{j,k} = (1 + j + k)^\gamma$$

that gelation occurs if $\lambda > 1$ and $\gamma < \frac{\lambda - 3}{2}$ where $\lambda = \alpha + \beta$. Gelation also occurs if initial conditions are sufficiently large, $\lambda > 1$ and $\frac{\lambda-3}{2} \leq \gamma < \lambda - 2$. There is no gelation if $\lambda > 1$ and $\gamma > \lambda - 2$ which loosely defines strong fragmentation.

The case when $\alpha = \beta = 1$ and $\gamma = 0$ (which corresponds to $K_{j,k} = 2jk$ and $L_{j,k} = 1$), is a borderline case in Escobedo et al. [9] and whether gelation occurs or not is unknown. Because of this, there is particular interest about the gelation phenomenon for general kernels, $K_{j,k} = \rho^2 jk$ and $L_{j,k} = b$ where ρ and b are real constants. Brunelle et al. [5] proved analytically for $K_{j,k} = \rho^2 jk$ and $b = \epsilon \rho^2 M_1$, where M_1 is total pre-gelation mass, that mass is conserved for $\epsilon \geq 6$. For smaller ϵ, a numerical approach suggests gelation time also tends to infinity. One of the goals in this thesis is to attempt a more analytical approach to determining gelation time.

1.1 Format of Thesis

In this thesis, the coagulation-fragmentation model will be solved for different cases of $K_{j,k} = A + B(j + k) + Cjk$ with $L_{j,k} = b \in \mathbb{R}_{\geq 0}$ and arbitrary initial condition. The main focus will be on three physical quantities: the total mass at time t, $M_1(t)$, the total number of clusters at t, $M_0(t)$, and the number of clusters at $t, N_k(t)$.

The first chapter explains the derivation of (1.2) and how to transform it into a PDE. Each of the next four chapters will investigate $M_1(t), M_0(t)$ and $N_k(t)$

of the coagulation-fragmentation PDE associated with one of the following coagulation kernels: the constant kernel, A, the sum kernel, $B(j+k)$, the constant-sum kernel, $A+B(j+k)$, and the product kernel, Cjk with b as the fragmentation kernel for each.

In the constant kernel chapter, an exact solution for $M_1(t)$ and $M_0(t)$ is easily determined. An inductive procedure is established to determine an exact formula for $N_k(t)$.

The sum kernel chapter is divided into two sections. The first discusses the solution to the coagulation model and the second is its corresponding coagulation-fragmentation model. Although the first section involves already published work [3], the results from the coagulation model are crucial for when fragmentation is added. An exact solution for $M_0(t)$ is readily found, determining $M_1(t)$ relies on [1] and an approximate formula for $N_k(t)$ is determined.

Similarly, the constant-sum kernel chapter is organized in the same way. The first section reproduces the results of the coagulation model [3] and the second section uses these results to solve its coagulation-fragmentation counterpart. Again, an exact solution for $M_0(t)$ is determined while a solution for $M_1(t)$ relies on [1] and an approximate formula for $N_k(t)$ is found.

The product kernel chapter is the most challenging but eminent model. The first section determines the solution for the coagulation model, which was first solved in [25]. In the second section, we extend the pre-gelation work of Brunelle et al. [5] by proving analytically that gelation time increases with the addition of fragmentation. A by-product of investigating gelation time are pre-gelation solutions to $M_1(t)$ and $M_0(t)$.

In the final chapter, a summary of the results for each model is reviewed. As well, a comparison of $M_0(t)$, $M_1(t)$ and $N_k(t)$ is discussed. Lastly, some future research avenues are suggested for the work begun in this thesis.

Chapter 2

Derivation of the Coagulation-Fragmentation Model

We are interested in a model that describes the rate of change of k size clusters. Clusters of size k can be created in two ways. The first is from small clusters coalescing to form one size k cluster. The second method is from a large cluster fragmenting into size k clusters. We must also take into account the formation of clusters with size not k. This can result by forming clusters of size greater than k or by breaking apart clusters of size less than k.

Let $j, k \in \mathbb{N}$. Denote

$N_k(t)$ as the number of size k clusters per unit volume at time $t \in [0, \infty)$,

$M_0(t)\left(= \sum_{k=1}^{\infty} N_k(t)\right)$ as the total number of clusters per unit volume at t,

$M_1(t)\left(= \sum_{k=1}^{\infty} kN_k(t)\right)$ as the total mass per unit volume at t,

$K_{j,k} :=$ coagulation kernel acting on clusters of size j and k,

$L_{j,k} :=$ fragmentation kernel acting on clusters of size j and k.

For physical reasons, $N_k(t), M_0(t)$ and $M_1(t)$ are assumed to be finite.

The total number of possible collisions between clusters of size j and $k-j$ is $N_j N_{k-j}$. Since $K_{j,k-j}$ is the rate at which they coalesce, the total number of coalescence from these collisions is $K_{j,k-j}N_jN_{k-j}$. Therefore, the total number of clusters of size k created in this manner is

$$\frac{1}{2}\sum_{j=1}^{k-1} K_{j,k-j}N_jN_{k-j}. \tag{2.1}$$

The factor of 1/2 is to avoid double counting since $N_jN_{k-j} = N_{k-j}N_j$.

Another way to form clusters of size k is through fragmentation. Since N_{j+k} is the total number of clusters of size $j+k$ and $L_{j,k}$ is the rate at which a size $j+k$ cluster can fragment into a cluster of size k, then the total number of clusters of size k formed in this manner is

$$\sum_{j=1}^{\infty} L_{j,k}N_{j+k}. \tag{2.2}$$

Meanwhile, clusters of size k can become bigger by coalescing with clusters of size j. The total number of clusters formed in this way is

$$\sum_{j=1}^{\infty} K_{j,k}N_jN_k. \tag{2.3}$$

And clusters of size k can fragment to form even smaller clusters. The total number of clusters created in this manner is

$$\frac{1}{2}\sum_{j=1}^{k-1} L_{j,k-j}N_k. \tag{2.4}$$

Combining (2.1), (2.2), (2.3), and (2.4), the rate of change of size k clusters can be modelled by

$$\begin{aligned}\frac{dN_k(t)}{dt} &= \frac{1}{2}\sum_{j=1}^{k-1} K_{j,k-j}N_jN_{k-j} - \sum_{j=1}^{\infty} K_{j,k}N_jN_k \\ &\quad + \sum_{j=1}^{\infty} L_{j,k}N_{j+k} - \frac{1}{2}\sum_{j=1}^{k-1} L_{j,k-j}N_k.\end{aligned} \tag{2.5}$$

This is an infinite system of nonlinear ODEs which can be transformed into a PDE by applying a generating function.

2.1 Deriving the PDE

From related literature, it is common to use a generating function to transform (2.5) into a PDE. Choosing the simplest generating function, $\phi(x,t) = \sum_{k=1}^{\infty} x^k N_k(t)$ for $x \in [0,1]$ and time, $t \in [0,\infty)$, will work nicely.

Differentiating $\phi(x,t)$ with respect to t,

$$\frac{\partial \phi(x,t)}{\partial t} = \sum_{k=1}^{\infty} x^k \frac{dN_k(t)}{dt} \tag{2.6}$$

and substituting (2.5) into (2.6),

$$\begin{aligned} \frac{\partial \phi(x,t)}{\partial t} = \sum_{k=1}^{\infty} x^k \Bigg[\frac{1}{2} \sum_{j=1}^{k-1} K_{j,k-j} N_j N_{k-j} - \sum_{j=1}^{\infty} K_{j,k} N_j N_k \\ + \sum_{j=1}^{\infty} L_{j,k} N_{j+k} - \frac{1}{2} \sum_{j=1}^{k-1} L_{j,k-j} N_k \Bigg]. \end{aligned} \tag{2.7}$$

Let the coagulation kernel be, $K_{j,k} = A + B(j+k) + Cjk$, and the fragmentation kernel be a constant, $L_{j,k} = b$, where A, B, C and b are positive real numbers. Substituting into (2.7),

$$
\begin{aligned}
\frac{\partial \phi(x,t)}{\partial t} &= \sum_{k=1}^{\infty} x^k \left[\frac{1}{2} \sum_{j=1}^{k-1} (A + Bk + Cj(k-j)) N_j N_{k-j} \right. \\
&\quad \left. - \sum_{j=1}^{\infty} (A + B(k+j) + Cjk) N_j N_k + \sum_{j=1}^{\infty} b N_{j+k} - \frac{1}{2} \sum_{j=1}^{k-1} b N_k \right] \\
&= A \left[\frac{1}{2} \sum_{k=1}^{\infty} x^k \sum_{j=1}^{k-1} N_j N_{k-j} - \sum_{k=1}^{\infty} x^k N_k \sum_{j=1}^{\infty} N_j \right] \\
&\quad + B \left[\frac{1}{2} \sum_{k=1}^{\infty} x^k \sum_{j=1}^{k-1} k N_j N_{k-j} - \sum_{k=1}^{\infty} x^k N_k \sum_{j=1}^{\infty} (k+j) N_j \right] \\
&\quad + C \left[\frac{1}{2} \sum_{k=1}^{\infty} x^k \sum_{j=1}^{k-1} j(k-j) N_j N_{k-j} - \sum_{k=1}^{\infty} x^k N_k \sum_{j=1}^{\infty} kj N_j \right] \\
&\quad + b \left[\sum_{k=1}^{\infty} x^k \sum_{j=1}^{\infty} N_{j+k} - \frac{1}{2} \sum_{k=1}^{\infty} x^k \sum_{j=1}^{k-1} N_k \right] \\
&= A \left[\frac{1}{2} \sum_{k=1}^{\infty} x^k N_k \sum_{j=1}^{\infty} x^j N_j - \sum_{k=1}^{\infty} x^k N_k \sum_{k=1}^{\infty} N_k \right] \\
&\quad + B \left[\sum_{k=1}^{\infty} x^k N_k \sum_{k=1}^{\infty} k x^k N_k - \sum_{k=1}^{\infty} k x^k N_k \sum_{k=1}^{\infty} N_k - \sum_{k=1}^{\infty} x^k N_k \sum_{k=1}^{\infty} k N_k \right] \\
&\quad + C \left[\frac{1}{2} \sum_{k=1}^{\infty} k x^k N_k \sum_{j=1}^{\infty} j x^j N_j - \sum_{k=1}^{\infty} k x^k N_k \sum_{k=1}^{\infty} k N_k \right] \\
&\quad + b \left[\sum_{i=1}^{\infty} \sum_{k=1}^{i-1} x^k N_i - \frac{1}{2} \sum_{k=1}^{\infty} x^k N_k (k-1) \right] \\
&= A \left[\frac{1}{2} \left(\sum_{k=1}^{\infty} x^k N_k \right)^2 - \sum_{k=1}^{\infty} x^k N_k \sum_{k=1}^{\infty} N_k \right] \\
&\quad + B \left[\left(\sum_{k=1}^{\infty} x^k N_k - \sum_{k=1}^{\infty} N_k \right) \sum_{k=1}^{\infty} k x^k N_k - \sum_{k=1}^{\infty} x^k N_k \sum_{k=1}^{\infty} k N_k \right] \\
&\quad + C \left[\frac{1}{2} \left(\sum_{k=1}^{\infty} k x^k N_k \right)^2 - \sum_{k=1}^{\infty} k x^k N_k \sum_{k=1}^{\infty} k N_k \right] \\
&\quad + b \left[\sum_{i=1}^{\infty} N_i \frac{x - x^i}{1-x} + \frac{1}{2} \left(- \sum_{k=1}^{\infty} k x^k N_k + \sum_{k=1}^{\infty} x^k N_k \right) \right]. \qquad (2.8)
\end{aligned}
$$

with initial condition

$$w(v,0) = h(v) := \sum_{k=1}^{\infty} e^{-kv} N_k(0).$$

In this case we have

$$M_0(t) = w(0,t), \qquad M_0(0) = h(0) =: h_0, \tag{2.13}$$

$$M_1(t) = -\frac{\partial w(0,t)}{\partial v}, \qquad M_1(0) = -h'(0) =: -h'_0. \tag{2.14}$$

Remark 2.1.

$$h(v) = h''(v) = \sum_{k=1}^{\infty} e^{-kv} N_k(0) \quad \Rightarrow \quad h(v) > 0 \text{ and monotone decreasing,}$$

$$h'(v) = -\sum_{k=1}^{\infty} k e^{-kv} N_k(0) \quad \Rightarrow \quad h'(v) < 0 \text{ and monotone increasing.}$$

The $\phi(x,t)$ generating function will be used to solve $K_{j,k} = A$ (constant kernel) while the $w(v,t)$ generating function will be used to solve $K_{j,k} = B(j+k)$ (sum kernel), $K_{j,k} = A + B(j+k)$ (constant-sum kernel) and $K_{j,k} = Cjk$ (product kernel). Deciding on which generating function to use is based on related literature, trial and error which leads to the last factor, previous experience.

Once $\phi(x,t)$ is known, the number of k size clusters at time t is described as

$$N_k(t) = \frac{1}{k!} \frac{\partial^k \phi}{\partial x^k}\bigg|_{x=0} \tag{2.15}$$

by applying Taylor series expansion to $\phi(x,t)$. From the definition of $\phi(x,t)$, it is clear $\partial^k \phi / \partial x^k$ exists for all k.

Chapter 3

Coagulation-Fragmentation Model with Constant Kernel

The pure coagulation model (i.e. $L_{j,k} = 0$) with constant kernel, $K_{j,k} = 1$, and a monodisperse initial condition, $h(x) = x$, was first solved by Smoluchowski [23, 24] in the early 1900s. In this chapter, fragmentation is added to Smoluchowski's coagulation model (that is, $L_{j,k} = b > 0$). Our contribution to his research is deriving the corresponding formula for $N_k(t)$ which is original work.

For $A, b > 0, B = C = 0$, (2.9) becomes

$$\frac{\partial \phi(x,t)}{\partial t} + \frac{b}{2} x \frac{\partial \phi}{\partial x} = A\left[\frac{1}{2}\phi^2 - \phi M_0\right] + b\left[\frac{1}{2}\phi + \frac{\phi - xM_0}{x-1}\right] \tag{3.1}$$

with the initial condition $\phi(x,0) = h(x)$. The method of characteristics will be used to solve this quasilinear PDE. Let $z = \phi$ and introduce the parameters, s and ξ. Consider the corresponding characteristic equations

$$\frac{dt}{ds} = 1, \qquad t(\xi, 0) = 0. \tag{3.2}$$

Clearly, $t = s$.

$$\frac{dx}{dt} = \frac{1}{2} bx, \qquad x(\xi, 0) = \xi. \tag{3.3}$$

By the method of separation of variables,

$$x(\xi, t) = \xi e^{\frac{1}{2}bt}. \tag{3.4}$$

$$\frac{dz}{dt} = A\left[\frac{1}{2}z^2 - M_0 z\right] + b\left[\frac{1}{2}z + \frac{z - xM_0}{x-1}\right], \qquad z(\xi, 0) = h(\xi). \tag{3.5}$$

Remark 3.1. Define $\xi = \hat{\xi}(x,t)$ to be the inverse function of $x = X(\xi, t)$ provided $\partial X(\xi,t)/\partial\xi \neq 0$. With the exception of the constant kernel case, $\hat{\xi}(x,t)$ is not known explicitly. This definition will be used throughout this thesis.

Before solving (3.5), $M_1(t)$ and $M_0(t)$ must be determined. Since $M_1(t) = \partial\phi(1,t)/\partial x$ by (2.11), then logically we would differentiate (3.1) with respect to x and evaluate x at 1 to determine $M_1(t)$.

$$\begin{aligned}\frac{dM_1(t)}{dt} &= AM_0(t)M_1(t) - AM_0(t)M_1(t)\\ &\quad + b\left[-\frac{1}{2}\frac{\partial^2\phi(1,t)}{\partial x^2} + \lim_{x\to 1}\frac{(\frac{\partial\phi}{\partial x} - M_0(t))(x-1) - \phi(x,t) + xM_0(t)}{(x-1)^2}\right]\end{aligned}$$

by substituting in (2.10) and (2.11). Using l'Hôpital's rule to evaluate the limit,

$$\frac{dM_1(t)}{dt} = 0 \Leftrightarrow \frac{\partial^2\phi}{\partial x^2}(1,t) < \infty$$

which means

$$M_1(t) = m \text{ for } t < t_g$$

where $m\,(= h_1'$ by (2.11)) is a positive real number and

$$t_g := \sup\{t \in (0,\infty] \mid \frac{\partial^2\phi}{\partial x^2}(1,t) < \infty\}. \tag{3.6}$$

Lemma 3.1. *$M_1(t) = m$ for all t (i.e. $t_g = \infty$).*

<u>Proof</u>

Since $\phi(x,t) = z(\hat{\xi}(x,t),t)$ by Remark 3.1, then

$$\frac{\partial\phi(x,t)}{\partial x} = \frac{\partial z(\hat{\xi}(x,t),t)}{\partial\xi}\frac{\partial\hat{\xi}(x,t)}{\partial x} = \frac{\frac{\partial z(\hat{\xi}(x,t),t)}{\partial\xi}}{\frac{\partial X(\hat{\xi}(x,t),t)}{\partial\xi}}.$$

The last equality comes from differentiating $x = X(\hat{\xi}(x,t),t)$ with respect to x. If $x = 1$ and $\partial X(\hat{\xi}(1,t),t)/\partial\xi \neq 0$, then

$$M_1(t) = \frac{\frac{\partial z(\hat{\xi}(1,t),t)}{\partial \xi}}{\frac{\partial X(\hat{\xi}(1,t),t)}{\partial \xi}}.$$

Since $\partial X(\hat{\xi}(1,t),t)/\partial\xi = e^{\frac{1}{2}bt} > 0$ for all t, then $M_1(t)$ is well-defined for all $t \in [0,\infty)$ (i.e. no shocks exist). Thus, $M_1(t) = m$ for all t which means there is conservation of mass in the system for all time. □

This supports the mass conservation results of Theorem 3.6 in Ball and Carr [1].

Remark 3.2. If $t_g \neq \infty$, then gelation occurs. Historically, the concept for the proof in Lemma 3.1 originates from Ziff and Stell [26] who described gelation as the formation of a shock wave solution.

Since $M_0(t) = \phi(1,t)$, to determine $M_0(t)$, evaluate $x = 1$ for (3.1) and substitute in $M_1(t) = m$,

$$\frac{dM_0}{dt} = \dot{M}_0(t) = -\frac{A}{2}{M_0}^2 - \frac{b}{2}M_0 + \frac{b}{2}m.$$

This is a Riccati Equation which is separable and integrable. If $M_0(t) \neq a_1, a_2$, rewrite it as

$$\frac{\dot{M}_0(t)}{(M_0 - a_1)(M_0 - a_2)} = -\frac{A}{2}$$

where

$$a_1 = -\frac{b}{2A} + \frac{1}{2}\sqrt{\frac{b^2}{A^2} + \frac{4bm}{A}}, \tag{3.7}$$

$$a_2 = -\frac{b}{2A} - \frac{1}{2}\sqrt{\frac{b^2}{A^2} + \frac{4bm}{A}}. \tag{3.8}$$

Applying partial fraction decomposition and then integrating with the initial condition, $M_0(0) = h_1$,

$$M_0(t) = \frac{a_1(h_1 - a_2) - a_2(h_1 - a_1)e^{-\frac{A}{2}(a_1 - a_2)t}}{h_1 - a_2 - (h_1 - a_1)e^{-\frac{A}{2}(a_1 - a_2)t}} \tag{3.9}$$

which is a special case of equation (13) in Brunelle et al. [5]. Since $a_2 < 0$ and $M_0(t)$ represents a physical quantity, then the only non-permissible value is $M_0(t) \neq a_1$. Furthermore, the only time $M_0(t) = a_1$ is at $t = \infty$ and $h_1 = a_1$.

From (3.9), for the pure coagulation model, that is, $b = 0$,

$$M_0(t) = \frac{2h_1}{Ah_1 t + 2}.$$

In the presence of only coagulation, $\lim_{t\to\infty} M_0(t) = 0$ while with the addition of fragmentation, $\lim_{t\to\infty} M_0(t) = a_1 > 0$. This is to be expected because during coagulation clusters can only aggregate to form larger clusters thus decreasing the number of clusters until eventually none are left. While fragmentation counteracts the growth of clusters and the emptying of the system observed in pure coagulation does not occur. As well, the leading behaviour of $M_0(t)$ for the coagulation and coagulation-fragmentation model is $2/At$ and $M_0(t) \sim a_1 + \frac{(h_1-a_1)(a_1-a_2)}{h_1-a_2} e^{-\frac{A}{2}(a_1-a_2)t}$ where $(a_1 - a_2) > 0$, respectively. It is interesting to note that both leading behaviours have decay rates but faster decay when fragmentation is present.

We are now ready to solve (3.5), but finding an exact solution is difficult. Instead, consider the following alternate approach.

$$\begin{aligned}
& \phi(x,t) = z(xe^{-\frac{1}{2}bt}, t) \quad \text{by (3.4)} \\
\Rightarrow \quad & \frac{\partial \phi}{\partial x}(x,t) = \frac{\partial z}{\partial \xi}(xe^{-\frac{1}{2}bt}, t)e^{-\frac{1}{2}bt} \\
\Rightarrow \quad & \frac{\partial^2 \phi}{\partial x^2}(x,t) = \frac{\partial^2 z}{\partial \xi^2}(xe^{-\frac{1}{2}bt}, t)e^{-bt} \\
& \vdots \\
\Rightarrow \quad & \frac{\partial^j \phi}{\partial x^j}(x,t) = \frac{\partial^j z}{\partial \xi^j}(xe^{-\frac{1}{2}bt}, t)e^{-\frac{j}{2}bt}, \quad j \in \mathbb{N}
\end{aligned}$$

Then

$$N_j(t) = \frac{1}{j!}\frac{\partial^j z}{\partial \xi^j}(0,t)e^{-\frac{j}{2}bt} = \frac{1}{j!} f_j(t) e^{-\frac{j}{2}bt} \quad \text{by (2.15)} \tag{3.10}$$

where for all j

$$f_j(t) = \frac{\partial^j z}{\partial \xi^j}(0,t)$$

and since $z(\xi,0) = h(\xi)$, the initial conditions are

$$f_j(0) = h^{(j)}(0) =: f_{j0} \quad \Rightarrow \quad N_j(0) = \frac{1}{j!} f_{j0}.$$

Ultimately, only $N_j(t)$ is of interest, thus it is sufficient to just find a formula for $f_j(t)$ instead of attempting to solve (3.5).

To begin deriving an expression for $f_j(t)$, differentiate (3.5) with respect to ξ,

$$\frac{\partial}{\partial \xi}\left(\frac{\partial z}{\partial t}\right) = Az\frac{\partial z}{\partial \xi} - AM_0\frac{\partial z}{\partial \xi} + b\left[\frac{1}{2}\frac{\partial z}{\partial \xi} + \frac{(\frac{\partial z}{\partial \xi} - e^{\frac{bt}{2}}M_0(t))(\xi e^{\frac{bt}{2}} - 1) - e^{\frac{bt}{2}}(z - \xi e^{\frac{bt}{2}}M_0(t))}{(\xi e^{\frac{bt}{2}} - 1)^2}\right]$$

after substituting in (3.4). Upon differentiating several times, a pattern emerges. Writing in general form, the suggested pattern for $j = 1$ is,

$$\frac{\partial}{\partial \xi}\frac{\partial z}{\partial t} + (AM_0 - \frac{b}{2})\frac{\partial z}{\partial \xi} = Az\frac{\partial z}{\partial \xi} + b\left[\frac{(\frac{\partial z}{\partial \xi} - M_0 e^{\frac{bt}{2}})}{(\xi e^{\frac{bt}{2}} - 1)} - \frac{(z - M_0 \xi e^{\frac{bt}{2}})e^{\frac{bt}{2}}}{(\xi e^{\frac{bt}{2}} - 1)^2}\right]$$

(3.11)

and for $j \in \mathbb{N}_{\geq 2}$ is,

$$\frac{\partial^j}{\partial \xi^j}\frac{\partial z}{\partial t} + (AM_0 - \frac{b}{2})\frac{\partial^j z}{\partial \xi^j} =$$

$$\begin{cases} A\sum_{n=1}^{\frac{j-1}{2}} \binom{j}{n} \frac{\partial^n z}{\partial \xi^n}\frac{\partial^{j-n} z}{\partial \xi^{j-n}} + Az\frac{\partial^j z}{\partial \xi^j} + b\left[\frac{\partial^j z}{\partial \xi^j}\frac{1}{\xi e^{\frac{bt}{2}}-1} + \sum_{n=2}^{j-1}\frac{(-1)^{j-n}\frac{j!}{n!}\frac{\partial^n z}{\partial \xi^n}e^{\frac{(j-n)bt}{2}}}{(\xi e^{\frac{bt}{2}}-1)^{j-n+1}} \right. \\ \left. + \frac{(-1)^{j+1}j!(\frac{\partial z}{\partial \xi} - M_0 e^{\frac{bt}{2}})e^{\frac{(j-1)bt}{2}}}{(\xi e^{\frac{bt}{2}}-1)^j} + \frac{(-1)^j j!(z - M_0\xi e^{\frac{bt}{2}})e^{\frac{jbt}{2}}}{(\xi e^{\frac{bt}{2}}-1)^{j+1}}\right], \quad j \text{ odd} \\ A\sum_{n=1}^{\frac{j-2}{2}} \binom{j}{n} \frac{\partial^n z}{\partial \xi^n}\frac{\partial^{j-n} z}{\partial \xi^{j-n}} + A\binom{j-1}{j/2}\left(\frac{\partial^{j/2} z}{\partial \xi^{j/2}}\right)^2 + Az\frac{\partial^j z}{\partial \xi^j} \\ +b\left[\frac{\partial^j z}{\partial \xi^j}\frac{1}{\xi e^{\frac{bt}{2}}-1} + \sum_{n=2}^{j-1}\frac{(-1)^{j-n}\frac{j!}{n!}\frac{\partial^n z}{\partial \xi^n}e^{\frac{(j-n)bt}{2}}}{(\xi e^{\frac{bt}{2}}-1)^{j-n+1}} \right. \\ \left. + \frac{(-1)^{j+1}j!(\frac{\partial z}{\partial \xi} - M_0 e^{\frac{bt}{2}})e^{\frac{(j-1)bt}{2}}}{(\xi e^{\frac{bt}{2}}-1)^j} + \frac{(-1)^j j!(z - M_0\xi e^{\frac{bt}{2}})e^{\frac{jbt}{2}}}{(\xi e^{\frac{bt}{2}}-1)^{j+1}}\right], \quad j \text{ even} \end{cases}$$

(3.12)

We now prove the veracity of Equation 3.12.

<u>Proof</u> (by induction)

Step 1: Show the $j = 2$ case is true.

Differentiating (3.5) twice with respect to ξ,

$$\frac{\partial^2}{\partial \xi^2}\frac{\partial z}{\partial t} = A\left(\frac{\partial z}{\partial \xi}\right)^2 + Az\frac{\partial^2 z}{\partial \xi^2} - AM_0\frac{\partial^2 z}{\partial \xi^2}$$
$$+ b\left[\frac{1}{2}\frac{\partial^2 z}{\partial \xi^2} + \frac{\frac{\partial^2 z}{\partial \xi^2}}{(\xi e^{\frac{bt}{2}}-1)} - 2\frac{(\frac{\partial z}{\partial \xi} - M_0 e^{\frac{bt}{2}})e^{\frac{bt}{2}}}{(\xi e^{\frac{bt}{2}}-1)^2} + 2\frac{(z - M_0\xi e^{\frac{bt}{2}})e^{\frac{bt}{2}}}{(\xi e^{\frac{bt}{2}}-1)^3}\right].$$

On the other hand, from (3.12)

$$\frac{\partial^2}{\partial \xi^2}\frac{\partial z}{\partial t} + (AM_0 - \frac{b}{2})\frac{\partial^2 z}{\partial \xi^2} = A\left(\frac{\partial z}{\partial \xi}\right)^2 + Az\frac{\partial^2 z}{\partial \xi^2}$$
$$+ b\left[\frac{\frac{\partial^2 z}{\partial \xi^2}}{(\xi e^{\frac{bt}{2}}-1)} + 0 - 2!\frac{(\frac{\partial z}{\partial \xi} - M_0 e^{\frac{bt}{2}})e^{\frac{bt}{2}}}{(\xi e^{\frac{bt}{2}}-1)^2} + 2!\frac{(z - M_0\xi e^{\frac{bt}{2}})e^{\frac{bt}{2}}}{(\xi e^{\frac{bt}{2}}-1)^3}\right].$$

Both expressions are identical, therefore, the $j = 2$ case is true.

Step 2: Assume the $j = k$ case is true.
(i.e. assume (3.12) is true).

Step 3: Show the $k+1$ case is true.
Assume k is odd $\Rightarrow k+1$ is even. Differentiate the assumption in Step 2 with respect to ξ,

$$\begin{aligned}
&\frac{\partial^{k+1}}{\partial\xi^{k+1}}\frac{\partial z}{\partial t} + (AM_0 - \frac{b}{2})\frac{\partial^{k+1} z}{\partial \xi^{k+1}} = A\sum_{n=1}^{\frac{k-1}{2}}\binom{k}{n}\left[\frac{\partial^{n+1} z}{\partial\xi^{n+1}}\frac{\partial^{k-n} z}{\partial\xi^{k-n}} + \frac{\partial^{n} z}{\partial\xi^{n}}\frac{\partial^{k-n+1} z}{\partial\xi^{k-n+1}}\right] \\
&+ A\frac{\partial z}{\partial\xi}\frac{\partial^k z}{\partial\xi^k} + Az\frac{\partial^{k+1} z}{\partial\xi^{k+1}} + b\left[\frac{\partial^{k+1} z}{\partial\xi^{k+1}}\frac{1}{\xi e^{\frac{bt}{2}}-1} - \frac{\partial^{k} z}{\partial\xi^{k}}\frac{e^{\frac{bt}{2}}}{(\xi e^{\frac{bt}{2}}-1)^2}\right. \\
&+ \sum_{n=2}^{k-1}(-1)^{k-n}\frac{k!}{n!}\left[\frac{\frac{\partial^{n+1} z}{\partial\xi^{n+1}}e^{\frac{(k-n)bt}{2}}}{(\xi e^{\frac{bt}{2}}-1)^{k+1-n}} - \frac{\frac{\partial^{n} z}{\partial\xi^{n}}e^{\frac{(k-n+1)bt}{2}}(k+1-n)}{(\xi e^{\frac{bt}{2}}-1)^{k+2-n}}\right] \\
&+ (-1)^{k+1}k!\frac{\partial^2 z}{\partial\xi^2}\frac{e^{\frac{(k-1)bt}{2}}}{(\xi e^{\frac{bt}{2}}-1)^{k}} - \frac{(-1)^{k+1}k!\left(\frac{\partial z}{\partial\xi} - M_0 e^{\frac{bt}{2}}\right)e^{\frac{kbt}{2}}k}{(\xi e^{\frac{bt}{2}}-1)^{k+1}} \\
&\left.+\frac{(-1)^{k}k!\left(\frac{\partial z}{\partial\xi} - M_0 e^{\frac{bt}{2}}\right)e^{\frac{kbt}{2}}}{(\xi e^{\frac{bt}{2}}-1)^{k+1}} - \frac{(k+1)(-1)^k k!\left(z - M_0\xi e^{\frac{bt}{2}}\right)e^{\frac{(k+1)bt}{2}}}{(\xi e^{\frac{bt}{2}}-1)^{k+2}}\right].
\end{aligned}$$

Recall the well known combinations identity,

$$\binom{k}{n} = \binom{k+1}{n} - \binom{k}{n-1}.$$

This identity and its proof can be found in [13] on page 36. Substituting in this identity and grouping like terms, the $k+1$ equation is recovered. (For a detailed explanation, please refer to Appendix A.) That is,

$$\begin{aligned}
&\frac{\partial^{k+1}}{\partial\xi^{k+1}}\frac{\partial z}{\partial t} + (AM_0 - \frac{b}{2})\frac{\partial^{k+1} z}{\partial \xi^{k+1}} = A\sum_{n=1}^{\frac{k-1}{2}}\binom{k+1}{n}\frac{\partial^{n} z}{\partial\xi^{n}}\frac{\partial^{k+1-n} z}{\partial\xi^{k+1-n}} + A\binom{k}{\frac{k+1}{2}}\left(\frac{\partial^{\frac{k+1}{2}} z}{\partial\xi^{\frac{k+1}{2}}}\right)^2 \\
&+ Az\frac{\partial^{k+1} z}{\partial\xi^{k+1}} + b\left[\frac{\partial^{k+1} z}{\partial\xi^{k+1}}\frac{1}{\xi e^{\frac{bt}{2}}-1} + \sum_{n=2}^{k}\frac{(-1)^{k+1-n}\frac{(k+1)!}{n!}\frac{\partial^{n} z}{\partial\xi^{n}}e^{\frac{(k+1-n)bt}{2}}}{(\xi e^{\frac{bt}{2}}-1)^{k-n+2}}\right. \\
&\left.+ \frac{(-1)^{k+2}(k+1)!(\frac{\partial z}{\partial\xi} - M_0 e^{\frac{bt}{2}})e^{\frac{kbt}{2}}}{(\xi e^{\frac{bt}{2}}-1)^{k+1}} + \frac{(-1)^{k+1}(k+1)!(z - M_0\xi e^{\frac{bt}{2}})e^{\frac{(k+1)bt}{2}}}{(\xi e^{\frac{bt}{2}}-1)^{k+2}}\right].
\end{aligned}$$

The even case can be derived in a similar manner. Therefore, by the principle of mathematical induction, (3.12) is true. □

Looking at (3.11) and (3.12), everything is known except for z. The following Lemma will be essential in resolving this obstacle.

Lemma 3.2. $z(0,t) = 0$ *for all* $t \in [0, \infty)$.

Proof

$$z(\xi,t) = \phi(xe^{\frac{-bt}{2}}, t) \text{ since } x(\xi,t) = \xi e^{\frac{1}{2}bt}$$
$$\Rightarrow z(0,t) = \phi(0,t) = \sum_{k=1}^{\infty} 0^k N_k(t) = 0. \qquad \square$$

We now have all the results necessary to derive expressions for $f_j(t)$.

For $j = 1$, evaluating $\xi = 0$ into (3.11) and applying Lemma 3.2,

$$\dot{f}_1(t) + (AM_0(t) + \frac{b}{2})f_1(t) = bM_0(t)e^{\frac{bt}{2}}, \quad f_1(0) = f_{01} \tag{3.13}$$

where $\dot{f}_1(t) = df_1(t)/dt$. This notation will be occasionally used throughout this thesis.

For $j \in \mathbb{N}_{\geq 2}$, evaluating $\xi = 0$ into (3.12) and applying Lemma 3.2,

$$\dot{f}_j(t) + (AM_0(t) + \frac{b}{2})f_j(t) =$$
$$\begin{cases} A\sum_{n=1}^{\frac{j-1}{2}} \binom{j}{n} f_n f_{j-n} - b\sum_{n=2}^{j-1} \frac{j!}{n!} f_n e^{\frac{(j-n)bt}{2}} \\ -bj![f_1(t) - M_0(t)e^{\frac{bt}{2}}]e^{\frac{(j-1)bt}{2}}, & j \text{ odd} \\ A\sum_{n=1}^{\frac{j-1}{2}} \binom{j}{n} f_n f_{j-n} + A\binom{j-1}{j/2} f_{j/2}^2 - b\sum_{n=2}^{j-1} \frac{j!}{n!} f_n e^{\frac{(j-n)bt}{2}} \\ -bj![f_1(t) - M_0(t)e^{\frac{bt}{2}}]e^{\frac{(j-1)bt}{2}}, & j \text{ even} \end{cases}$$

(3.14)

with the initial conditions $f_j(0) = f_{j0}$.

Using the integrating factor,

$$\mu(t) = (h_1 - a_2 - (h_1 - a_1)e^{\frac{-A(a_1-a_2)t}{2}})^2 e^{\frac{A(a_1-a_2)t}{2}}, \quad \mu(0) = (a_1 - a_2)^2$$

to solve (3.13),

$$\begin{aligned} f_1(t) = & \frac{f_{10}(a_1 - a_2)^2}{\mu(t)} + \frac{b}{A\mu(t)} \Big[2(a_2 - h_1)(a_1 - h_1)(e^{\frac{b}{2}t} - 1) \\ & - \frac{a_1}{a_2}(a_2 - h_1)^2(e^{-Aa_2t} - 1) - \frac{a_2}{a_1}(a_1 - h_1)^2(e^{-Aa_1t} - 1) \Big]. \end{aligned} \tag{3.15}$$

To solve (3.14) will be much more involved. First notice, all the ODEs have $\mu(t)$ as its integrating factor, which means proving the integrals,

$$f_j(t)\mu(t) - f_{j0}(a_1 - a_2)^2 =$$
$$\begin{cases} A\sum_{n=1}^{\frac{j-1}{2}} \binom{j}{n} \int_0^t f_n f_{j-n}\mu d\bar{t} - b\sum_{n=2}^{j-1} \frac{j!}{n!} \int_0^t f_n e^{\frac{(j-n)b\bar{t}}{2}} \mu d\bar{t} \\ -bj! \int_0^t [f_1(t) - M_0(t)e^{\frac{b\bar{t}}{2}}] e^{\frac{(j-1)b\bar{t}}{2}} \mu d\bar{t}, & j \text{ odd} \\ A\sum_{n=1}^{\frac{j-1}{2}} \binom{j}{n} \int_0^t f_n f_{j-n}\mu d\bar{t} + A\binom{j-1}{j/2} \int_0^t f_{j/2}^2 \mu d\bar{t} \\ -b\sum_{n=2}^{j-1} \frac{j!}{n!} \int_0^t f_n e^{\frac{(j-n)b\bar{t}}{2}} \mu d\bar{t} - bj! \int_0^t [f_1(\bar{t}) - M_0(\bar{t})e^{\frac{b\bar{t}}{2}}] e^{\frac{(j-1)b\bar{t}}{2}} \mu d\bar{t}, \\ & j \text{ even} \end{cases} \tag{3.16}$$

exist is sufficient in proving (3.14) can be solved. This will be done using a proof by (strong) induction since the integrals from (3.16) are of f_n where $n < j$.

Prove the integrals of (3.16) exist.

Proof (sketch)

By strong induction, we assume the integrals of (3.16) exist for $j = 1, 2, .., k$ which means they are continuous for $[0, t]$, $t \in (0, \infty)$. These continuous integrals become the continuous integrands for the $k + 1$ case. Since these integrands are continuous on $[0, t]$, then their integrals exist on the same interval. □

A more detailed proof can be found in Appendix B.

Therefore, by (3.10) and (3.16) a formula for the number of j size clusters at time t is

$$N_j(t) = \frac{e^{-\frac{j}{2}bt}}{j!\mu(t)} f_{j0}(a_1 - a_2)^2 +$$
$$\begin{cases} \frac{e^{-\frac{j}{2}bt}}{j!\mu(t)} \left[A \sum_{n=1}^{\frac{j-1}{2}} \binom{j}{n} \int_0^t f_n f_{j-n} \mu d\bar{t} - b \sum_{n=2}^{j-1} \frac{j!}{n!} \int_0^t f_n e^{\frac{(j-n)b\bar{t}}{2}} \mu d\bar{t} \right. \\ \left. -bj! \int_0^t [f_1(t) - M_0(t) e^{\frac{b\bar{t}}{2}}] e^{\frac{(j-1)b\bar{t}}{2}} \mu d\bar{t} \right], & j \text{ odd} \\ \frac{e^{-\frac{j}{2}bt}}{j!\mu(t)} \left[A \sum_{n=1}^{\frac{j-1}{2}} \binom{j}{n} \int_0^t f_n f_{j-n} \mu \bar{t} + A \binom{j-1}{j/2} \int_0^t f_{j/2}^2 \mu \bar{t} \right. \\ \left. -b \sum_{n=2}^{j-1} \frac{j!}{n!} \int_0^t f_n e^{\frac{(j-n)b\bar{t}}{2}} \mu d\bar{t} - bj! \int_0^t [f_1(\bar{t}) - M_0(\bar{t}) e^{\frac{b\bar{t}}{2}}] e^{\frac{(j-1)b\bar{t}}{2}} \mu d\bar{t} \right], \\ & j \text{ even} \end{cases}$$

(3.17)

To the best of our knowledge, (3.17), which describes the behaviour of any size j cluster in a coagulation-fragmentation model with constant coagulation and fragmentation kernels and arbitrary initial condition, is an original result.

A simple example of $N_j(t)$ for $j = 1, 2, 3$ with a monodisperse initial condition will now be considered. This example recovers the particular solution determined in Blatz and Tobolsky [4] after rescaling their fragmentation kernel by 1/2.

Example 3.1. To determine the simplest $N_j(t)$ for $j = 1, 2, 3$, let $A = b = 1$ and $h(x) = x$ (monodisperse initial condition) which implies $h_1 = h(1) = 1$ and $m = h_1' = h'(1) = 1$. Thus, by (3.9)

$$M_0(t) = \frac{a_1(1 - a_2) - a_2(1 - a_1)e^{-\frac{1}{2}(a_1 - a_2)t}}{1 - a_2 - (1 - a_1)e^{-\frac{1}{2}(a_1 - a_2)t}}$$

	$\lim_{t\to\infty}$
$M_0(t)$	$\frac{1}{2}+\frac{\sqrt{5}}{2}=0.6180$
$N_1(t)$	$\frac{3}{2}-\frac{\sqrt{5}}{2}=0.3820$
$N_2(t)$	$\frac{7}{2}-3\frac{\sqrt{5}}{2}=0.1459$
$N_3(t)$	$9-4\sqrt{5}=0.0557$

Table 3.1: $\lim_{t\to\infty} M_0(t), N_j(t)$ for $j=1,2,3$.

where by (3.7) and (3.8)

$$a_1=-\frac{1}{2}+\frac{1}{2}\sqrt{5} \quad \text{and} \quad a_2=-\frac{1}{2}-\frac{1}{2}\sqrt{5}.$$

And by (3.15) and (3.16)

$$\begin{aligned}
f_1(t)=&\frac{1}{\mu(t)}\left[2e^{\frac{1}{2}t}-\frac{(-1+\sqrt{5})(3+\sqrt{5})^2(e^{\frac{1}{2}(1+\sqrt{5})t}-1)}{4(1+\sqrt{5})}\right.\\
&\left.+\frac{(1+\sqrt{5})(-3+\sqrt{5})^2(e^{\frac{1}{2}(1-\sqrt{5})t}-1)}{4(-1+\sqrt{5})}+3\right],\\
f_2(t)=&\frac{1}{\mu(t)}\left[(5\sqrt{5}+11)e^t+2e^{-\frac{1}{2}(\sqrt{5}-2)t}+2e^{\frac{1}{2}(\sqrt{5}+2)t}+\frac{10(15+7\sqrt{5})e^t}{-7-3\sqrt{5}+2e^{-\frac{\sqrt{5}}{2}t}}\right],\\
f_3(t)=&\frac{1}{\mu(t)}\left[(60\sqrt{5}+132)e^{\frac{3}{2}t}+(9-3\sqrt{5})e^{\frac{1}{2}(3+\sqrt{5})t}+(9+3\sqrt{5})e^{\frac{1}{2}(3-\sqrt{5})t}\right.\\
&\left.-\frac{60}{11}\frac{(95+43\sqrt{5})(26+10\sqrt{5}-11e^{-\frac{\sqrt{5}}{2}t})}{(-7-3\sqrt{5}+2e^{-\frac{\sqrt{5}}{2}t})^2}e^{\frac{3}{2}t}\right]
\end{aligned}$$

where

$$\mu(t)=\frac{1}{4}\left(3+\sqrt{5}-(3-\sqrt{5})e^{-\frac{\sqrt{5}}{2}t}\right)^2 e^{\frac{\sqrt{5}}{2}t}.$$

Therefore by (3.10)

$$N_1(t)=f_1(t)e^{-\frac{t}{2}}, \quad N_2(t)=\frac{1}{2}f_2(t)e^{-t} \quad \text{and} \quad N_3(t)=\frac{1}{6}f_3(t)e^{-\frac{3}{2}t}.$$

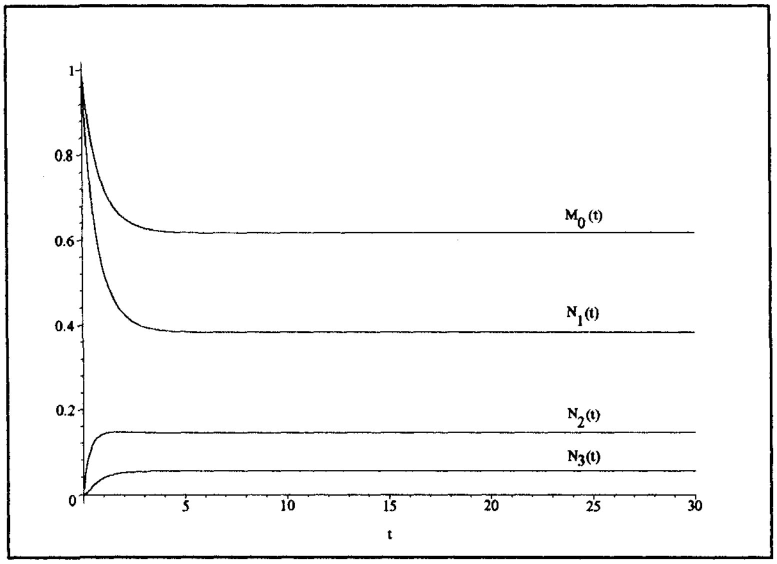

Figure 3.1: Graphical representation of $M_0(t)$ and $N_j(t)$ for $j = 1, 2, 3$.

From the positive limits in Table 3.1, it is clear that $M_0(t), N_1(t), N_2(t)$ and $N_3(t)$ support the earlier result that clusters are present for all time when fragmentation is present. From Figure 3.1, it is clear $M_0(t), N_1(t), N_2(t)$ and $N_3(t)$, which are physical quantities, are greater than zero with $M_0(t)$ greater than $N_1(t), N_2(t)$ and $N_3(t)$ since $M_0(t)$ represents the total number of clusters. As well, $M_0(0) = N_1(0) = 1$ and $N_2(0) = N_3(0) = 0$ corroborates with the monodisperse initial condition.

With a monodisperse initial condition, $N_1(t)$ initially decreases while $N_2(t)$ is increasing because size 1 clusters coalesce to form size 2 clusters, soon though fragmentation begins and the opposing processes eventually reach a positive equilibrium. The shape of $N_3(t)$ also supports this observation. Another interesting observation is $N_1(t) > N_2(t) \geq N_3(t)\ \forall\ t \geq 0$. In other words, the bigger the clusters the less of them there are. Physically this makes sense since it takes more small clusters to make just one bigger cluster.

Remark 3.3. By letting $b = 0$ in this chapter, the pure coagulation case can be recovered.

Chapter 4

Coagulation-Fragmentation Model with Sum Kernel

4.1 Coagulation Model

In 1986, Lu [3] solved the pure coagulation model with sum kernel $K_{j,k} = j+k$ and an arbitrary initial condition. He transformed (1.1) into one term and then applied an exponential generating function, one which is different from $w(v,t)$, to solve the associated PDE. In order to solve the coagulation-fragmentation case, solutions from the pure coagulation model are required; therefore, a modified version of Lu's work is reproduced below. Instead of initially applying a transformation, (2.12) will be used with a general sum kernel, $K_{j,k} = B(i+j)$.

For $B > 0, A = C = b = 0$, (2.12) becomes

$$\frac{\partial w}{\partial t} - B(M_0 - w)\frac{\partial w}{\partial v} = -BwM_1 \tag{4.1}$$

with initial condition $w(v,0) = h(v)$. The method of characteristics will be used to solve this quasilinear PDE. Letting $z = w$ and introducing the parameters, s and ξ, the characteristic equations are

$$\frac{dt}{ds} = 1, \qquad t(0,\xi) = 0. \tag{4.2}$$

Clearly, $t = s$.

$$\frac{dv}{dt} = -B(M_0 - z), \qquad v(0,\xi) = \xi. \tag{4.3}$$

$$\frac{dz}{dt} = -BM_1 z, \qquad z(0,\xi) = h(\xi). \tag{4.4}$$

Before solving (4.3) and (4.4), $M_1(t)$ and $M_0(t)$ must be determined.

Using the same technique from Chapter 3 to determine $M_1(t)$,

$$M_1(t) = m \text{ for } t < t_g$$

where $m\,(= -h_0'$ by (2.14)) is a positive real number and t_g defined by (3.6). Shirvani and van Roessel's 1992 paper [16] proved $M_1(t) = m$ for all t. In the constant model, conservation of mass for all time was directly proven by relying on $\partial v/\partial\xi$ (refer to Lemma 3.1). That cannot be used here because $v(\xi,t)$ depends on $M_1(t)$. For the same reason, Lemma 3.1 cannot be applied to any of the other models.

Using the same technique from Chapter 3 to determine $M_0(t)$,

$$M_0(t) = h_0 e^{-Bmt}$$

for all t with the initial condition $M_0(0) = h_0$. Since $Bmt \geq 0$, then clearly $M_0(t)$ has an exponential decay and $\lim_{t\to\infty} M_0(t) = 0$. In the constant coagulation model, $M_0(t)$ also has a decay rate but it is of algebraic form and $\lim_{t\to\infty} M_0(t) = 0$.

With $M_0 = h_0 e^{-Bmt}$ and $M_1 = m$, it is clear the solutions to the characteristic equations are

$$z(\xi,t) = h(\xi)e^{-Bmt}, \tag{4.5}$$

$$v(\xi,t) = -\frac{h(\xi) - h_0}{m}(e^{-Bmt} - 1) + \xi. \tag{4.6}$$

No further pure coagulation results are required for the coagulation-fragmentation model.

4.2 Coagulation-Fragmentation Model

In this section, fragmentation will be added to Lu's coagulation results with the sum kernel (that is, $K_{j,k} = B(j+k)$ and $L_{j,k} = b$). Our goal is to solve the corresponding PDE which leads to formulas for $N_k(t), M_0(t)$ and $M_1(t)$. Determining a formula for $N_k(t)$ is original work.

For $A = C = 0, B > 0$ and $b = \epsilon B > 0$, (2.12) becomes

$$\frac{\partial w}{\partial t} - B\left[(M_0 - w) + \frac{\epsilon}{2}\right]\frac{\partial w}{\partial v} = -BM_1 w + \epsilon B\left[\frac{1}{2}w + \frac{w - M_0 e^{-v}}{e^{-v} - 1}\right] \tag{4.7}$$

with the initial condition $w(v,0) = h(v)$. The method of characteristics will be used to solve this quasilinear PDE. Letting $z = w$ and introducing the parameters, s and ξ, the characteristic equations are

$$\frac{dt}{ds} = 1, \qquad t(\xi, 0) = 0. \tag{4.8}$$

Clearly, $t = s$.

$$\frac{dv}{dt} = -B(M_0 - z) - \frac{\epsilon B}{2}, \qquad v(\xi, 0) = \xi. \tag{4.9}$$

$$\frac{dz}{dt} = -BM_1 z + \epsilon B\left[\frac{1}{2} + \frac{z - M_0 e^{-v}}{e^{-v} - 1}\right], \qquad z(\xi, 0) = h(\xi). \tag{4.10}$$

Before solving (4.9) and (4.10), $M_1(t)$ and $M_0(t)$ must be determined.

Using the same technique from Chapter 3 to determine $M_1(t)$ and $M_0(t)$,

$$M_1(t) = m,$$
$$M_0(t) = \frac{\epsilon m}{2m + \epsilon} + \left(h_0 - \frac{\epsilon m}{2m + \epsilon}\right) e^{-B(m + \frac{\epsilon}{2})t}$$

for $t < t_g$ where m is a positive real number and t_g defined by (3.6). In Ball and Carr's 1989 paper ([1], Theorem 3.6), they proved $M_1(t) = m$ for all t. Therefore, the above equations for $M_1(t)$ and $M_0(t)$ are valid for all t. A continuous version of $M_0(t)$ can be found in [2].

Remark 4.1. A neat way to check whether $M_0(t)$ is correct is by setting $\epsilon = 0$ and recovering $M_0(t)$ for the coagulation case. This check can be used for all the remaining cases.

Recall in the coagulation case, $M_0(t) = h_0 e^{-Bmt}$ and with the addition of fragmentation, $M_0(t) = \frac{\epsilon}{2m+\epsilon} + (h_0 - \frac{\epsilon m}{2m+\epsilon})e^{-B(m+\frac{\epsilon}{2})t}$ where $B(m + \frac{\epsilon}{2})t > 0$. Both equations for $M_0(t)$ decay exponentially but faster when fragmentation is present. Also, as $t \to \infty$, the limits for $M_0(t)$ are 0 in the coagulation case and $\frac{\epsilon m}{2m+\epsilon} > 0$ (i.e. some clusters remain in the system) in the coagulation-fragmentation model. Similar observations for the constant model were also noted.

Finding an exact solution for (4.10) is difficult. For the constant kernel case, determining z relied on explicitly knowing $x(\xi, t)$ (which corresponds to $v(\xi, t)$ in this chapter). But that method cannot be applied here because $dv/d\xi$ depends on z. Instead, the solution can be approximated by considering a regular perturbation expansion about $\epsilon > 0$,

$$z = \sum_{n=0}^{\infty} z_n(\xi, t)\epsilon^n.$$

Furthermore, the leading behaviour of the solution can be approximated from just the first two terms of this series. In other words,

$$z \approx z_0 + \epsilon z_1.$$

Similarly,

$$v \approx v_0 + \epsilon v_1,$$

$$M_0 \approx M_{00} + \epsilon M_{01},$$

$$M_1 \approx M_{10} + \epsilon M_{11}.$$

Exact solutions for M_0 and M_1 are known, which means M_{00}, M_{01}, M_{10} and M_{11} are all known. Therefore, the problem becomes determining v_0, v_1, z_0 and z_1. Since v_0 and z_0 are solutions for $\epsilon = 0$ (i.e. $b = 0$), it has already been solved in Section 4.1. That is, from (4.6),

$$v_0(\xi, t) = \frac{h(\xi) - h_0}{m}(1 - e^{-Bmt}) + \xi \tag{4.11}$$

and from (4.5),

$$z_0(\xi, t) = h(\xi)e^{-Bmt}. \tag{4.12}$$

Thus the problem reduces to just finding z_1 and v_1.

To determine z_1, consider approximating (4.10) so that

$$\begin{aligned} \frac{dz_0}{dt} + \epsilon\frac{dz_1}{dt} &\approx -B(M_{10}(t) + \epsilon M_{11}(t) - \frac{\epsilon}{2})(z_0 + \epsilon z_1) \\ &\quad + \epsilon B\left[\frac{(z_0 + \epsilon z_1) - e^{-(v_0+\epsilon v_1)}(M_{00} + \epsilon M_{01})}{e^{-(v_0+\epsilon v_1)} - 1}\right]. \end{aligned} \tag{4.13}$$

Expanding and considering only order ϵ terms,

$$\begin{aligned} \frac{dz_1}{dt} + BM_{10}z_1 &= BM_{11}z_0 + \frac{B}{2}z_0 + B\left[\frac{z_0 - M_{00}e^{-v_0}}{e^{-v_0} - 1}\right] \\ &= BM_{11}z_0 + \frac{B}{2}(z_0 - 2M_{00}) + B\left[\frac{z_0 - M_{00}}{e^{-v_0} - 1}\right], \qquad z_1(\xi, 0) = 0 \end{aligned} \tag{4.14}$$

In a similar manner, the approximation for v_1 is

$$\frac{dv_1}{dt} = -B(M_{01}(t) - z_1) - \frac{B}{2}, \qquad v_1(\xi, 0) = 0. \tag{4.15}$$

By series expanding $M_0(t)$ and $M_1(t)$,

$$\begin{aligned} M_{00}(t) &= h_0e^{-Bmt}, \\ M_{01}(t) &= \frac{1}{2} - \frac{1}{2}Bh_0e^{-Bmt}t - \frac{1}{2}e^{-Bmt}, \\ M_{10}(t) &= m, \\ M_{11}(t) &= 0. \end{aligned}$$

Series expanding $M_0(t)$ was done on Maple.

Remark 4.2. $M_{00}(t)$ is identical to the coagulation case which it should be. As well, $\lim_{t\to\infty} M_{00}(t)+\epsilon M_{01}(t) = \frac{\epsilon}{2}$ while $\lim_{t\to\infty} M_0(t) = \frac{\epsilon m}{2m+\epsilon} \sim \frac{\epsilon}{2}$ by series expanding around ϵ. These simple verifications can be used on the other cases as well.

By applying the integrating factor, $\psi(\xi,t) = e^{Bmt}$ on (4.14),

$$z_1(\xi,t) = \frac{B}{2}(h(\xi) - 2h_0)te^{-Bmt} + Be^{-Bmt}F(\xi,t)$$

where

$$F(\xi,t) = \int_0^t \frac{h(\xi)-h_0}{e^{-v_0(\xi,\bar{t})}-1}d\bar{t}, \quad v_0(\xi,\bar{t}) = \frac{h(\xi)-h_0}{m}(1-e^{-Bm\bar{t}})+\xi$$

for all $t \in [0,\infty)$ and $\xi \in [0,\infty)$

We now prove $F(\xi,t)$ exists for $t \in [0,\infty)$ with $\xi \in [0,\infty)$ fixed.

Proof

Case $1 : \xi > 0,\ t > 0$

If $v_0(\xi,\bar{t}) \neq 0$ for all $t \Rightarrow$ the integrand is continuous, then $F(\xi,t)$ exists.

From Remark 2.1, $h'(\xi)$ is continuous and monotone increasing implies $h'(0) < h'(c)$ for all $c > 0$. By the Mean Value Theorem, there exists a $c \in (0,\xi)$ such that $h'(c) = \frac{h(\xi)-h(0)}{\xi}$

$$\Rightarrow h'(0) < \frac{h(\xi)-h(0)}{\xi}$$

$$\Rightarrow 1 > -\frac{h(\xi)-h(0)}{\xi m}, \quad m = -h'(0) > 0 \text{ and } h \text{ is decreasing by Remark 2.1}$$

$$\Rightarrow -1 < \frac{h(\xi)-h(0)}{\xi m}(1-e^{-Bm\bar{t}}) \quad \text{since } -1 < (e^{-Bm\bar{t}}-1) < 0,\ Bm > 0$$

$$\Rightarrow 0 < \frac{h(\xi)-h_0}{m}(1-e^{-Bm\bar{t}}) + \xi = v_0(\xi,\bar{t}).$$

Therefore, $v_0(\xi,\bar{t}) \neq 0 \Rightarrow F(\xi,t)$ exists.

Case $2 : \xi = 0,\ t > 0$

If $\xi = 0$, then

$$F(0,t) = -h_0'\int_0^t e^{Bm\bar{t}}d\bar{t} = m\int_0^t e^{Bm\bar{t}}d\bar{t} \quad \text{since} \quad m = -h_0'$$

by the Dominated Convergence Theorem. Solving the integral,

$$F(0,t) = \frac{(e^{Bmt} - 1)}{B}.$$

Case 3 : $\xi \geq 0,\ t = 0 \Rightarrow F(\xi, t) = 0.$ □

With $z_1(\xi, t)$ known, (4.15) is determined to be

$$\begin{aligned} v_1(\xi,t) =& -Bt - \frac{B}{2m}(h(\xi) - h_0)te^{-Bmt} - \frac{1}{2m}\left(\frac{h(\xi) - h_0}{m} - 1\right)(e^{-Bmt} - 1) \\ &+ B^2(h(\xi) - h_0)\int_0^t e^{-Bmr}F(\xi, r)dr \end{aligned}$$

We have now found the leading order solution to (4.7),

$$\begin{aligned} w(v,t) \approx& z_0(\hat{\xi}(v,t),t) + \epsilon z_1(\hat{\xi}(v,t),t) \\ =& h(\hat{\xi}(v,t))e^{-Bmt} \\ &+ \epsilon\left(\frac{B}{2}(h(\hat{\xi}(v,t)) - 2h_0)te^{-Bmt} + Be^{-Bmt}F(\hat{\xi}(v,t),t)\right) \end{aligned} \tag{4.16}$$

for $t \in [0, \infty)$ with $\hat{\xi}(v, t)$ (defined in Remark 3.1) determined from $v(\xi, t) \approx v_0(\xi, t) + \epsilon v_1(\xi, t)$. By (2.15), we have an implicit approximation for $N_k(t)$, which to our knowledge is an original result.

Chapter 5

Coagulation-Fragmentation Model with Constant-Sum Kernel

5.1 Coagulation Model

Lu [3] is also credited with solving the pure coagulation model with a constant-sum kernel, $K_{j,k} = A + B(i+j)$, and arbitrary initial condition. Once again he transformed equation (1.1) into one term and then applied the ϕ generating function. To determine the coagulation-fragmentation model, solutions from the coagulation model are again needed. Thus, Lu's work will be recreated but without applying a transformation.

For $A, B > 0, C = b = 0$, the PDE, (2.12), becomes

$$\frac{\partial w}{\partial t} - B(M_0 - w)\frac{\partial w}{\partial v} = \frac{A}{2}w^2 - (AM_0 + BM_1)w \tag{5.1}$$

with the initial condition $w(v, 0) = h(v)$. The method of characteristics will be used to solve this quasilinear PDE. Letting $z = w$ and introducing the parameters, s and ξ, the characteristic equations are

$$\frac{dt}{ds} = 1, \qquad t(0,\xi) = 0. \tag{5.2}$$

Clearly, $t = s$.

$$\frac{dv}{dt} = -B(M_0 - z), \qquad v(0,\xi) = \xi. \tag{5.3}$$

$$\frac{dz}{dt} = \frac{A}{2}z^2 - (AM_0 + BM_1)z, \qquad z(0,\xi) = h(\xi). \tag{5.4}$$

Before solving (5.3) and (5.4), $M_1(t)$ and $M_0(t)$ must be determined.

Using the same technique from Chapter 3 to determine $M_1(t)$ and $M_0(t)$,

$$M_1(t) = m \text{ for } t < t_g$$

where m is a positive real number and t_g defined by (3.6). By Shirvani and van Roessel's theorem [16], $M_1(t) = m$ for all t. With this result

$$M_0(t) = \frac{2h_0Bm}{(2Bm + Ah_0)e^{Bmt} - Ah_0}$$

for all t with the initial condition $M_0(0) = h_0$.

$M_0(t)$ has an exponential decay and $\lim_{t\to\infty} M_0(t) = 0$ which are identical results to the sum model. The observation, $\lim_{t\to\infty} M_0(t) = 0$, has now occurred in all three different cases of the coagulation model. As well, in this model $M_0(t) \sim \frac{2h_0Bm}{2Bm+Ah_0}e^{-Bmt}$. A decay rate for the leading order behaviour of $M_0(t)$ has now occurred in all three models.

With $M_0(t)$ and $M_1(t)$ known, (5.4), which is a Bernoulli equation, and (5.3) are determined to be

$$z(\xi,t) = \frac{(2Bm)^2h(\xi)e^{-Bmt}}{(2Bm + Ah_0(1 - e^{-Bmt}))(2Bm + A(h_0 - h(\xi)(1 - e^{-Bmt}))}, \tag{5.5}$$

$$v(\xi,t) = \xi - \frac{2B}{A}\ln\left(1 + \frac{A}{2Bm}(h_0 - h(\xi))(1 - e^{-Bmt})\right). \tag{5.6}$$

Absolute values are not required for ln because $A, B, m > 0$ and $h(\xi)$ decreasing by Remark 2.1 implies $1 + \frac{A}{2Bm}(h_0 - h(\xi))(1 - e^{-Bmt}) > 0$ all $t \geq 0$.

Remark 5.1. In this remark, the verification idea of Remark 4.1 is extended. By setting $A = 0$ (or $B = 0$), $M_0(t)$ for the sum (or constant) coagulation model can be recovered. This is a good way to check whether $M_0(t)$ was correctly determined. In fact, $v(\xi, t)$ and $z(\xi, t)$ can be verified in an identical fashion.

No further pure coagulation results are required for the coagulation-fragmentation model.

5.2 Coagulation-Fragmentation Model

In this section, fragmentation will be added to Lu's pure coagulation results with the constant-sum kernel (that is, $K_{j,k} = A + B(j+k)$ and $L_{j,k} = b$). Our goal is to solve the corresponding PDE which leads to formulas for $N_k(t), M_0(t)$ and $M_1(t)$. Determining a formula for $N_k(t)$ is original work.

For $A, B > 0$, $C = 0$ and $b = \epsilon AB > 0$, (2.12) becomes

$$\frac{\partial w}{\partial t} - B\left[(M_0 - w) + \frac{\epsilon A}{2}\right]\frac{\partial w}{\partial v} = \frac{A}{2}w^2 - AM_0 w - BM_1 w + \epsilon AB\left[\frac{1}{2}w + \frac{w - M_0 e^{-v}}{e^{-v} - 1}\right] \tag{5.7}$$

with the initial condition $w(v, o) = h(v)$. The method of characteristics will be used to solve this quasilinear PDE. Letting $z = w$ and introducing the parameters, s and ξ, the characteristic equations are

$$\frac{dt}{ds} = 1, \qquad t(\xi, 0) = 0. \tag{5.8}$$

Clearly, $t = s$.

$$\frac{dv}{dt} = -B(M_0 - z) - \frac{\epsilon AB}{2}, \qquad v(\xi, 0) = \xi. \tag{5.9}$$

$$\frac{dz}{dt} = \frac{A}{2}z^2 - (AM_0 + BM_1)z + \epsilon AB\left[\frac{1}{2} + \frac{w - M_0 e^{-v}}{e^{-v} - 1}\right], \qquad z(\xi, 0) = h(\xi). \tag{5.10}$$

Before solving (5.10), $M_1(t)$ and $M_0(t)$ must be determined.

Applying the method from Chapter 3 to determine $M_1(t)$ and $M_0(t)$,

$$\begin{aligned} M_1(t) &= m, \\ M_0(t) &= \frac{a_1(h_0 - a_2) - a_2(h_0 - a_1)e^{-\frac{A}{2}(a_1-a_2)t}}{h_0 - a_2 - (h_0 - a_1)e^{-\frac{A}{2}(a_1-a_2)t}} \end{aligned}$$

for $t < t_g$ where m is a positive real number, t_g defined by (3.6) and

$$\begin{aligned} a_1 &= -\frac{B}{A}\left(m + \frac{\epsilon A}{2}\right) + \sqrt{\frac{B^2}{A^2}\left(m + \frac{\epsilon A}{2}\right)^2 + \epsilon B m}, \\ a_2 &= -\frac{B}{A}\left(m + \frac{\epsilon A}{2}\right) - \sqrt{\frac{B^2}{A^2}\left(m + \frac{\epsilon A}{2}\right)^2 + \epsilon B m}. \end{aligned}$$

Ball and Carr's paper ([1], Theorem 3.6) proved $M_1(t) = m$ for all t; therefore, the above equations for $M_1(t)$ and $M_0(t)$ are true for all t. A continuous version of $M_0(t)$ can be found in [2].

We see $\lim_{t\to\infty} M_0(t) = a_1 > 0$ and $M_0(t) \sim a_1 + \frac{(h_0-a_1)(a_1-a_2)}{h_0-a_2} e^{\frac{-A}{2}(a_1-a_2)t}$ where $(a_1 - a_2) > 0$. It is apparent with the addition of fragmentation clusters remain in the system as $t \to \infty$. The leading behaviour of $M_0(t)$ is again an exponential decay. Furthermore, $M_0(t)$ with fragmentation decays faster than its coagulation counterpart. These same observations were noted in both the constant and sum model.

Finding an exact solution for (5.10) is difficult. Instead, the approximation technique used in Section 4.2 will be applied here. Therefore,

$$\begin{aligned} \frac{dz_1}{dt} - (Az_0 - AM_{00} - BM_{10})z_1 &= -(AM_{01} + BM_{11})z_0 \\ &\quad + AB\left[\frac{1}{2}z_0 - M_{00} + \frac{z_0 - M_{00}}{e^{-v_0} - 1}\right], \qquad z_1(\xi, 0) = 0 \qquad (5.11) \end{aligned}$$

$$\frac{dv_1}{dt} = -B(M_{01} - z_{01} + \frac{A}{2}), \qquad v_1(\xi, 0) = 0 \qquad (5.12)$$

where

$$
\begin{aligned}
z_0(\xi,t) &= \frac{(2Bm)^2 h(\xi) e^{-Bmt}}{(2Bm + Ah_0(1-e^{-Bmt}))(2Bm + A(h_0 - h(\xi)(1-e^{-Bmt}))},\\
v_0(\xi,t) &= \xi - \frac{2B}{A}\ln\left(1 + \frac{A}{2Bm}(h_0 - h(\xi))(1-e^{-Bmt})\right),\\
M_{00}(t) &= \frac{2h_0 Bme^{-Bmt}}{2Bm + Ah_0(1-e^{-Bmt})},\\
M_{01}(t) &= \frac{\begin{array}{c}-A[Ah_0^2(A+2B)e^{-2Bmt} + 2B(A+B)h_0 m(Ah_0+2Bm)te^{-Bmt}\\ +2B(-Ah_0^2 + 2Ah_0 m + 2Bm^2)]\end{array}}{2(2Bm + Ah_0(1-e^{-Bmt}))^2},\\
M_{10}(t) &= m,\\
M_{11}(t) &= 0.
\end{aligned}
$$

Series expanding $M_0(t)$ was again done on Maple.

Applying the integrating factor, $\psi(\xi,t) = e^{Bmt}(1+\frac{A}{2Bm}(h_0 - h(\xi))(1-e^{-Bmt}))^2$ with $\psi(\xi,0)=1$, on (5.11)

$$
\begin{aligned}
z_1(\xi,t)\psi(\xi,t) =& -A\int_0^t M_{01} z_0 \psi d\bar{t} + AB\int_0^t \psi\left(\frac{1}{2}z_0 - M_{00}\right)d\bar{t}\\
&+ AB\int_0^t \psi \frac{z_0 - M_{00}}{e^{-v_0}-1} d\bar{t}.
\end{aligned} \tag{5.13}
$$

The first integral has an explicit solution but is extremely complicated because the coefficients have been left arbitrary. Once specific values are assigned the solution will simplify greatly. The second integral is easily and neatly solvable. The third integral cannot be explicitly solved and for convenience will be denoted as

$$
\begin{aligned}
G(\xi,t) =& AB\int_0^t \psi(\xi,\bar{t})\frac{z_0(\xi,\bar{t}) - M_{00}(\xi,\bar{t})}{e^{-v_0(\xi,\bar{t})}-1}d\bar{t}\\
=& AB(h(\xi)-h_0)\int_0^t \frac{1 + \frac{A(h_0 - h(\xi))}{2Bm}(1-e^{-Bm\bar{t}})}{e^{-\xi}(1+\frac{A(h_0-h(\xi))}{2Bm}(1-e^{-Bm\bar{t}}))^{\frac{2B}{A}} - 1}d\bar{t}.
\end{aligned}
$$

We now prove $G(\xi,t)$ exists $t \in [0,\infty)$ with $\xi \in [0,\infty)$ fixed.

<u>Proof</u>

Case $1 : \xi \neq 0$

If $e^{-\xi}(1+\frac{A(h_0-h(\xi))}{2Bm}(1-e^{-Bm\bar{t}}))^{\frac{2B}{A}}-1 \neq 0$ for all t then, $G(\xi,t)$ exists. Suppose not. Assume, there exists some $\bar{t}$ such that $e^{-\xi}(1+\frac{A(h_0-h(\xi))}{2Bm}(1-e^{-Bm\bar{t}}))^{\frac{2B}{A}}-1 = 0$. Isolating for $\bar{t}$,

$$\bar{t} = \frac{-1}{Bm}\ln\left(1-\frac{2Bm(e^{\frac{\xi A}{2B}}-1)}{A(h_0-h(\xi))}\right).$$

By the assumption and $Bm > 0$,

$$\ln\left(1-\frac{2Bm(e^{\frac{\xi A}{2B}}-1)}{A(h_0-h(\xi))}\right) \leq 0 \quad \Leftrightarrow \quad 0 < 1-\frac{2Bm(e^{\frac{\xi A}{2B}}-1)}{A(h_0-h(\xi))} \leq 1.$$

Considering $0 < 1-\frac{2Bm(e^{\frac{\xi A}{2B}}-1)}{A(h_0-h(\xi))}$, then

$\Rightarrow \frac{2Bm}{A}(e^{\frac{\xi A}{2B}}-1) < h_0 - h(\xi)$ since h is monotone decreasing by Remark 2.1

$\Rightarrow \frac{2Bm}{A\xi}(e^{\frac{\xi A}{2B}}-1) < \frac{-(h(\xi)-h_0)}{\xi} = -h'(c)$, by the Mean Value Theroem where $c \in (0,\xi)$

$\Rightarrow \frac{2Bm}{A\xi}(e^{\frac{\xi A}{2B}}-1) < -h_0'$ since h' is monotone decreasing by Remark 2.1

$\Rightarrow$ since $m = -h_0' > 0$, then $(e^k - 1) < k$ (*) where $k = \frac{\xi A}{2B} > 0$.

On the other hand, defining $f(k) = e^k - 1 - k \Rightarrow f'(k) = e^k - 1 > 0$ since $k > 0 \Rightarrow f$ is increasing for all $k > 0$. With $f(0) = 0$ and f increasing, then $f > 0 \Rightarrow e^k - 1 > k$ which contradicts (*).

Case $2 : \xi = 0$

If $\xi = 0$, then

$$G(0,t) = \int_0^t \frac{-ABh_0'm}{m+h_0'(1-e^{-Bm\bar{t}})}d\bar{t} = \int_0^t ABme^{-Bm\bar{t}}d\bar{t} \quad \text{since} \quad m = -h_0'$$

by the Dominated Convergence Theorem. Solving the integral,

$$G(0,t) = A(e^{Bmt}-1).$$

Therefore, $G(\xi,t)$ exists. □

Solving (5.13) on Maple,

$$z_1(\xi,t)\psi(\xi,t) \approx \frac{\begin{aligned}&\Big[-A\big\{h(\xi)(Ah_0+2Bm)(2B^2h(\xi)m(Ah_0+2Bm)\ln(2Bm)\\&+Ah_0[-2A(A+B)h_0(h_0-h(\xi))-B(3A+2B)(2h_0-h(\xi))m-4(Bm)^2])\\&+Bh(\xi)m(Ah_0+2Bm)^2([2Bm(Bh(\xi)+Ah_0)+A^2h_0(h_0-h(\xi))]t\\&-2Bh(\xi)\ln((Ah_0+2Bm)e^{Bmt}-Ah_0))\big\}e^{2Bmt}\\&+2A^2h_0\big\{2A^2(A+B)h_0^2h(\xi)(h(\xi)-h_0)-2AB(4A+3B)h_0^2h(\xi)m\\&-2B^2(2B+5A)h_0h(\xi)m^2+2B^2(2A+B)h^2(\xi)m^2+AB(6A+5B)h_0h^2(\xi)m\\&-4B^3h(\xi)m^3+2B^2h^2(\xi)m(Ah_0+2Bm)\ln(2Bm)\\&+B^2h(\xi)m(h(\xi)-h_0)(Ah_0+2Bm)^2t\\&-2B^2h^2(\xi)m(Ah_0+2Bm)\ln((Ah_0+2Bm)e^{Bmt}-Ah_0)\big\}e^{Bmt}\\&-A^3B(A+2B)h_0^2h(\xi)(h(\xi)-h_0)m(Ah_0+2Bm)t\\&+2A^3B^2h_0^2h^2(\xi)m\ \ln((Ah_0+2Bm)e^{Bmt}-Ah_0)\\&-A^3h_0h(\xi)\big\{2h_0(h(\xi)-h_0)(Ah_0(A+B)+2B^2m)+2B^2h_0h(\xi)m\ \ln(2Bm)\\&-Bm(2B(2h_0-h(\xi))m+Ah_0(6h_0-5h(\xi)))\big\}\Big]\end{aligned}}{2Bh_0m(Ah_0+2Bm)((Ah_0+2Bm)e^{Bmt}-Ah_0)^2}$$

$$-\frac{A^2(h_0-h(\xi))^2(e^{-Bmt}-1)}{2Bm^2}-\frac{ABh^2(\xi)}{h_0(2Bm+Ah_0)}\ln(1-\frac{Ah_0}{2Bm}(e^{-Bmt}-1))$$

$$-\frac{A\{A(h_0-h(\xi))+2Bm\}\{Bm(2h_0-h(\xi))+Ah_0(h_0-h(\xi))\}t}{2m(2Bm+Ah_0)}+G(\xi,t).$$

Absolute values are not required for ln since $Bm > 0$

$$\Rightarrow \quad Ah_0+2Bm > Ah_0$$

$$\Rightarrow \quad (Ah_0+2Bm)e^{Bmt} > Ah_0 \quad \text{since } e^{Bmt} \geq 1$$

$$\left(\text{which also implies } \Rightarrow 1 > \frac{Ah_0}{2Bm}(e^{-Bmt}-1)\right)$$

for all $t \geq 0$. As well, this proves $\ln((Ah_0+2Bm)e^{Bmt}-Ah_0)$ is continuous for all t. Furthermore, $1/\psi(\xi,t)$ is also continuous for all t since h is monotone decreasing by Remark 2.1 and $1-e^{-Bmt} > 0$,

$$\Rightarrow \quad (1+\frac{A}{2Bm}(h_0-h(\xi))(1-e^{-Bmt}))^2 \geq 1$$

$$\Rightarrow \quad \psi(\xi,t)=e^{Bm\bar{t}}(1+\frac{A}{2Bm}(h_0-h(\xi))(1-e^{-Bmt}))^2 > 0$$

for all t. Therefore, $z_1(\xi,t)$ is continuous for all t.

With $z_1(\xi,t)$ known, (5.12) is calculated to be

$$\begin{aligned}
v_1(\xi,t) &= -B\int_0^t M_{01}d\bar{t}+B\int_0^t z_1 d\bar{t}-\frac{AB}{2}t \\
&= -\left[\frac{A}{2}+B+\frac{AB}{2}\right]t+\frac{(A+B)(Ah_0+2B,)te^{Bmt}}{(2Bm+Ah_0)e^{Bmt}-Ah_0} \\
&+\frac{2A(Ah_0+Bh_0+Bm)}{Ah_0+2Bm}\left[\frac{1}{(2Bm+Ah_0)e^{Bmt}-Ah_0}-\frac{1}{2Bm}\right]+B\int_0^t z_1 d\bar{t}
\end{aligned}$$

While the first integral is easily solved, the second cannot be completely determined but since $z_1(\xi,t)$ is continuous for all $t \in [0,\infty)$ then its integral exists.

We have now found a leading order solution to the coagulation-fragmentation model, (5.7),

$$w(v,t) \approx z_0(\hat{\xi}(v,t),t)+\epsilon z_1(\hat{\xi}(v,t),t)$$

for $t \in [0,\infty)$ with $\hat{\xi}(v,t)$ (defined in Remark 3.1) determined from $v(\xi,t) \approx v_0(\xi,t)+\epsilon v_1(\xi,t)$. By (2.15), we have found an implicit approximation for $N_k(t)$, which to our knowledge is an original result.

Chapter 6

Coagulation-Fragmentation Model with Product Kernel

6.1 Coagulation Model

The pure coagulation model for $K_{j,k} = jk$ with an arbitrary initial condition was solved for all time by Ziff et al. [25]. They solved the model using a slightly different generating function than $w(v,t)$. We reproduce the work of Ziff et al. using $w(v,t)$ because the results are needed in Section 6.2.

For $C > 0$ and $A = B = b = 0$, the PDE, (2.12), becomes

$$\frac{\partial w(v,t)}{\partial t} - CM_1 \frac{\partial w}{\partial v} = C\frac{1}{2}\left(\frac{\partial w}{\partial v}\right)^2 \tag{6.1}$$

with the initial condition $w(v,0) = h(v)$. The method of characteristics will be used to solve this nonlinear PDE. Letting $z = w, p = \partial w/\partial v, q = \partial w/\partial t$, (6.1) becomes

$$F(v,t,z,p,q) := q - C\left[\frac{1}{2}p^2 + pM_1\right].$$

And introducing the parameters, s and ξ, the characteristic equations are

$$\frac{dt}{ds} = \frac{\partial F}{\partial q} = 1, \qquad t(\xi, 0) = 0. \tag{6.2}$$

Clearly, $t = s$.

$$\frac{dv}{dt} = \frac{\partial F}{\partial p} = -C(p + M_1), \qquad v(\xi, 0) = \xi. \tag{6.3}$$

$$\frac{dz}{dt} = p\frac{\partial F}{\partial p} + q\frac{\partial F}{\partial q} = -Cp(p + M_1) + q, \qquad z(\xi, 0) = h(\xi). \tag{6.4}$$

$$\frac{dp}{dt} = -\frac{\partial F}{\partial v} - p\frac{\partial F}{\partial z} = 0, \qquad p(\xi, 0) = h'(\xi). \tag{6.5}$$

$$\frac{dq}{dt} = -\frac{\partial F}{\partial t} - q\frac{\partial F}{\partial z} = -Cp\dot{M}_1, \; q(\xi, 0) = C\left[\frac{1}{2}(h'(\xi))^2 - h'(\xi)h'_0\right] \tag{6.6}$$

where $h'_0 = M_1(0)$.

Clearly, first solving (6.5) is necessary in determining the other characteristic equations and luckily it is easily evaluated to be

$$p(\xi, t) = h'(\xi). \tag{6.7}$$

From this the remaining characteristic equations are determined to be

$$v(\xi, t) = -Ch'(\xi)t - C\int_0^t M_1(\bar{t})d\bar{t} + \xi, \tag{6.8}$$

$$z(\xi, t) = -\frac{C}{2}(h'(\xi))^2 t + h(\xi), \tag{6.9}$$

$$q(\xi, t) = Ch'(\xi)\left[M_1(t) + \frac{1}{2}h'(\xi)\right]. \tag{6.10}$$

Thus far, we have made no restrictions on t and therefore (6.7) to (6.10) are valid for all time. However, in order to determine explicit solutions for $v(\xi, t)$ and $q(\xi, t)$ requires knowing $M_1(t)$.

Using the same technique from Chapter 3 to determine $M_1(t)$ and $M_0(t)$,

$$\begin{aligned} M_1(t) =& m, \\ M_0(t) =& -\frac{C}{2}m^2 t + h_0, \qquad M_0(0) = h_0 \end{aligned}$$

for $t < t_g$ where m is a positive real number and t_g defined by (3.6). In Shirvani and van Roessel's paper [16], they proved $M_1(t) = m$ up to $t < t_g$ only. This means gelation occurs. At this point, we would usually compare $M_0(t)$ with the others from the previous cases. However, because of the gelation phenomenon, to make a comparison would not seem prudent.

Equations (6.8) and (6.10) are evaluated to be,

$$v(\xi, t) = -C(h'(\xi) + m)t + \xi \text{ for } t < t_g, \tag{6.11}$$

$$q(\xi, t) = Ch'(\xi)\left[m + \frac{1}{2}h'(\xi)\right] \text{ for } t < t_g, \tag{6.12}$$

while (6.7) and (6.9) are valid for all time.

Post-gelation results will not be determined as they are unnecessary for the next section.

Recall from Remark 3.2 that gelation corresponds to a shock in the solution of (6.1). A shock is characterized by $\partial w/\partial v$ becoming infinite or $\partial v/\partial \xi = 0$. Therefore, differentiating (6.8) and setting it equal to zero,

$$\frac{\partial v(\xi, t)}{\partial \xi} = -Ch''(\xi)t + 1 = 0.$$

The shock occurs at

$$t = \frac{1}{Ch''(\xi)} =: T_0(\xi) \tag{6.13}$$

and the first time it occurs is known as the gelation time,

$$t_{go} := \inf_{0 \le \xi < \infty} T_0(\xi) = \frac{1}{Ch''(0)}$$

since h'' is monotone decreasing by Remark 2.1.

To clarify the notation for gelation time, t_g is a generic gelation time while

$t_{g_0} :=$ gelation time for the pure coagulation model,

$t_{g_\epsilon} :=$ gelation time for the coagulation-fragmentation model.

6.2 Coagulation-Fragmentation Model

In this section, the gelation time for the coagulation-fragmentation model (that is, $K_{j,k} = Cjk$ and $L_{j,k} = b$) is investigated.

For $C > 0, A = B = 0$ and $b = \epsilon C > 0$, (2.12) becomes

$$\frac{\partial w}{\partial t} - C\left[M_1 + \frac{\epsilon}{2}\right]\frac{\partial w}{\partial v} = \frac{C}{2}\left(\frac{\partial w}{\partial v}\right)^2 + \epsilon B\left[\frac{1}{2}w + \frac{w - M_0 e^{-v}}{e^{-v} - 1}\right] \tag{6.14}$$

with the initial condition $w(v, 0) = h(v)$. The method of characteristics will be applied to this nonlinear PDE. Letting $z = w, p = \partial w/\partial v, q = \partial w/\partial t$ and introducing the parameters, s and ξ, the characteristic equations as illustrated in Section 6.1 are

$$\frac{dt}{ds} = 1, \qquad t(\xi, 0) = 0. \tag{6.15}$$

Clearly, $t = s$.

$$\frac{dv}{dt} = -C(p + M_1) - \frac{\epsilon C}{2}, \qquad v(\xi, 0) = \xi. \tag{6.16}$$

$$\frac{dz}{dt} = -Cp(p + M_1) - \frac{\epsilon C}{2}p + q, \qquad z(\xi, 0) = h(\xi). \tag{6.17}$$

$$\frac{dp}{dt} = \epsilon C\frac{e^{-v}(z - M_0)}{(e^{-v} - 1)^2} + \epsilon C\left[\frac{1}{2} + \frac{1}{e^{-v} - 1}\right]p, \qquad p(\xi, 0) = h'(\xi). \tag{6.18}$$

$$\frac{dq}{dt} = -Cp\dot{M}_1 + \epsilon C\left[\frac{q - e^{-v}\dot{M}_0}{e^{-v}-1} + \frac{q}{2}\right],$$

$$q(\xi,0) = C\left[\frac{1}{2}(h'(\xi))^2 - h'(\xi)h'_0\right] + \epsilon C\left[\frac{1}{2}(h(\xi)+h'(\xi)) + \frac{h(\xi)-h_0e^{-\xi}}{e^{-\xi}-1}\right]$$

(6.19)

where $h_0 = M_0(0)$ and $h'_0 = M_1(0)$.

Using the same technique from Chapter 3 to determine $M_1(t)$ and $M_0(t)$,

$$M_1(t) = m,$$
$$M_0(t) = m - \frac{m^2}{\epsilon} + (h_0 - m + \frac{m^2}{\epsilon})e^{-\frac{1}{2}\epsilon Ct}, \qquad M_0(0) = h_0$$

for $t < t_g$ where m is a positive real number and t_g defined by (3.6). The equation for $M_0(t)$ is a special case of equation 13 from Brunelle et al. [5]. And as discussed in Section 6.1, no comparison of $M_0(t)$ will be made.

At this point we would usually find a solution to (6.14). But due to the difficulties of finding a solution, we limit our investigation to gelation time. Brunelle et al. [5] proved numerically for the case of a monodisperse initial condition that gelation time tends to infinity for a critical value, ϵ_c. In the paper, $M_1(t)$ is computed to be constant for $t \in [0, 10)$. Then extrapolating at $t = 10$, $M_1(10)$ is no longer constant at $\epsilon \lessapprox 1.43 = \epsilon_c$. However, there still lacks a rigorous proof whether gelation occurs. Our contribution is to show analytically that gelation time for pure coagulation occurs earlier than when fragmentation is added (that is, $t_{g_0} < t_{g_\epsilon}$). Physically, this is because fragmentation counteracts the effect of coagulation therefore delaying the formation of a superparticle, which characterizes gelation.

Theorem 6.1. *$t_{g_0} < t_{g_\epsilon}$ for the case of a monodisperse initial condition*

Proof

The approximation technique from Section 4.2 will once again be called upon. However, since we are only interested in gelation time, we concentrate our approximation on

$$\frac{dv_1}{dt} = -Cp_1 - \frac{C}{2}, \qquad v_1(\xi,0)=0 \tag{6.20}$$

$$\frac{dp_1}{dt} = C\left[\frac{e^{-v_0}(z_0 - M_{00})}{(e^{-v_0}-1)^2} + \left(\frac{1}{2}+\frac{1}{e^{-v_0}-1}\right)p_0\right], \qquad p_1(\xi,0)=0 \tag{6.21}$$

where for $t < t_g$

$$z_0(\xi,t) = -\frac{1}{2}C(h'(\xi))^2 t + h(\xi), \tag{6.22}$$

$$v_0(\xi,t) = -C(h'(\xi)+m)t + \xi, \tag{6.23}$$

$$p_0(\xi,t) = h'(\xi), \tag{6.24}$$

$$M_{00}(t) = -\frac{1}{2}Cm^2 t + h_0. \tag{6.25}$$

Series expanding $M_0(t)$ was determined on Maple.

Since the right-hand side of (6.21) is known, integrating the ODE,

$$p_1(\xi,t) = -C\frac{b(\xi)}{a(\xi)}\frac{t}{e^{a(\xi)t-\xi}-1} - C\frac{h(\xi)-h_0}{a(\xi)}\left[\frac{1}{e^{a(\xi)t-\xi}-1} - \frac{1}{e^{-\xi}-1}\right]$$
$$+C\left(\frac{b(\xi)}{a^2(\xi)} + \frac{h'(\xi)}{a(\xi)}\right)\left[\ln|1-e^{-a(\xi)\bar{t}+\xi}| - \ln|1-e^{\xi}|\right] + \frac{C}{2}h'(\xi)t$$

for $t < t_g$ where

$$a(\xi) = C(h'(\xi) - h_0'),$$
$$b(\xi) = \frac{-1}{2}C((h'(\xi))^2 - m^2) = \frac{-1}{2}C(h'(\xi)-h_0')(h'(\xi)+h_0').$$

Therefore, (6.20) is

$$-\frac{v_1(\xi,t)}{C} = -C\frac{b(\xi)}{a^2(\xi)}\ln|1-e^{-a(\xi)t+\xi}|t + C\frac{m}{a(\xi)}F(\xi,t) - \frac{1}{2}\ln|1-e^{\xi}|t$$
$$-C\frac{h(\xi)-h_0}{a^2(\xi)}\left[\ln|1-e^{-a(\xi)\bar{t}+\xi}| - \ln|1-e^{\xi}|\right]$$
$$+C\frac{h(\xi)-h_0}{a(\xi)}\frac{t}{e^{-\xi}-1} + \frac{C}{4}h'(\xi)t^2 + \frac{t}{2} \tag{6.26}$$

for $t < t_g$ where

$$F(\xi,t) = \int_0^t \ln|1-e^{-a(\xi)\bar{t}+\xi}|\,d\bar{t}.$$

At $\bar{t}_d = \xi/a(\xi)$, $\ln|1 - e^{-a(\xi)\bar{t}+\xi}|$ is discontinuous. To remedy this, we rewrite $F(\xi, t)$ as an improper integral,

$$F(\xi,t) = \lim_{d \to \bar{t}_d} \left[\int_0^d \ln(e^{-a(\xi)\bar{t}+\xi} - 1)\, d\bar{t} + \int_d^t \ln(1 - e^{-a(\xi)\bar{t}+\xi})\, d\bar{t} \right].$$

In Section 6.1, to determine gelation time, we solved t for $dv(\xi,t)/dt = 0$. In this case, $v(\xi,t) \approx v_0(\xi,t) + \epsilon v_1(\xi,t)$ does not allow t to be isolated. Since our actual goal is to show $t_{g_0} < t_{g_\epsilon}$, it suffices to prove $T_1(\xi) > 0$ where $T(\xi,\epsilon) := T_0(\xi) + \epsilon T_1(\xi)$ (from Section 6.1, $T_0(\xi) = \frac{1}{Ch''(\xi)}$) such that

$$\frac{\partial v(\xi, T(\xi,\epsilon))}{\partial \xi} = 0.$$

Furthermore, since

$$\begin{aligned} \frac{\partial v(\xi, T(\xi,\epsilon))}{\partial \xi} &\approx \frac{\partial v_0(\xi, T(\xi,\epsilon))}{\partial \xi} + \epsilon \frac{\partial v_1(\xi, T(\xi,\epsilon))}{\partial \xi} \\ &= \frac{\partial v_0(\xi, T_0(\xi) + \epsilon T_1(\xi))}{\partial \xi} + \epsilon \frac{\partial v_1(\xi, T_0(\xi) + \epsilon T_1(\xi))}{\partial \xi}, \end{aligned}$$

then applying Taylor series expansion

$$\frac{\partial v_0(\xi, T_0(\xi))}{\partial \xi} + \epsilon \left[T_1(\xi) \frac{\partial^2 v_0(\xi, T_0(\xi))}{\partial \xi \partial t} + \frac{\partial v_1(\xi, T_0(\xi))}{\partial \xi} \right] \approx 0.$$

Since $\partial v_0/\partial \xi = 0$ (this is from determining gelation time for the pure coagulation model), this implies

$$T_1(\xi) \approx -\frac{\frac{\partial v_1(\xi, T_0(\xi))}{\partial \xi}}{\frac{\partial^2 v_0(\xi, T_0(\xi))}{\partial \xi \partial t}}. \tag{6.27}$$

Therefore, to prove $t_{g_0} < t_{g_\epsilon}$, we must show $T_1(\xi)$ given in (6.27) is greater than zero.

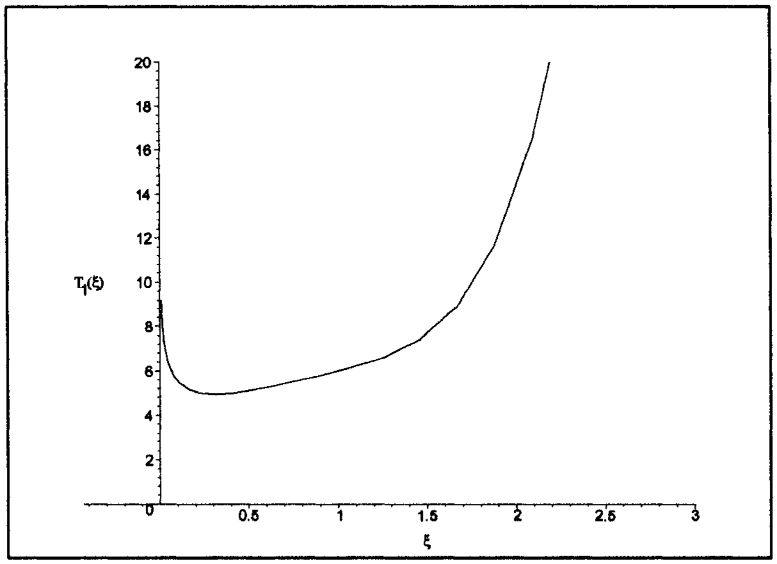

Figure 6.1: Graphical representation of $T_1(\xi)$.

By applying (6.26) and (6.23),

$$-\frac{\frac{\partial v_1(\xi,t)}{\partial \xi}}{\frac{\partial^2 v_0(\xi,t)}{\partial \xi \partial t}} = \frac{1}{(1-e^{-\xi})^2}\left[\left(-\frac{1}{2}(1+e^{-\xi})t+1\right)\ln|1-e^{(e^{-\xi}-1)t+\xi}| + F(\xi,t)\right.$$

$$\left. - \ln|1-e^{\xi}| + t\right] + \frac{e^{\xi}}{e^{-\xi}-1}\left[\frac{1}{2}e^{-\xi}\ln|1-e^{(e^{-\xi}-1)t+\xi}|t\right.$$

$$\left. - \frac{-\frac{1}{2}(1-e^{-\xi})t+1}{1-e^{(e^{-\xi}-1)t+\xi}}e^{(e^{-\xi}-1)t+\xi}(-e^{-\xi}t+1) + \frac{\partial F(\xi,t)}{\partial t} + \frac{e^{\xi}}{1-e^{\xi}}\right]$$

$$+\frac{e^{\xi}}{2(1-e^{-\xi})}t - \frac{1}{4}t^2 \tag{6.28}$$

where the arbitrary initial condition has been replaced with the monodisperse initial condition, $h(\xi) = e^{-\xi}$, and $C = 1$. Since $T_0(\xi) = e^{\xi}$ from (6.13) and by substituting (6.28) into (6.27), then

$$T_1(\xi) \approx \frac{2e^{\xi} - \ln(e^{\xi}-1)}{(e^{-\xi}-1)^2} + \frac{e^{2\xi}}{4}\left(\frac{1+e^{-\xi}}{1-e^{-\xi}}\right) + \frac{F(\xi,e^{\xi})}{(1-e^{-\xi})^2} + \frac{e^{\xi}}{e^{-\xi}-1}\frac{dF(\xi,e^{\xi})}{d\xi}$$

where

$$F(\xi,e^{\xi}) = \lim_{d\to\frac{\xi}{1-e^{-\xi}}}\left[\int_0^d \ln(e^{(e^{-\xi}-1)\bar{t}+\xi}-1)d\bar{t} + \int_d^{e^{\xi}} \ln(1-e^{(e^{-\xi}-1)\bar{t}+\xi})d\bar{t}\right].$$

Since it appears $T_1(0)$ is undefined, we consider $\xi > 0$ for $T_1(\xi)$. This means gelation time cannot occur at $\xi = 0$ and this will be validated once t_{g_ϵ} is known.

From Figure 6.1, $T_1(\xi)$ appears positive for all ξ. Since $T_1(\xi)$ has a critical value at $\xi = 0.3098$, $\lim_{\xi \to 0^+} T_1(\xi) = \lim_{\xi \to \infty} T_1(\xi) = \infty$ and $T_1(\xi)$ continuous for all $\xi > 0$, then $T_1(\xi)$ has an absolute minimum at $\xi = 0.3098$. Therefore, $T_1(\xi) > T_1(0.3098) \approx 4.94$ for all ξ.

Therefore, $t_{g_0} < t_{g_\epsilon}$ for $h(\xi) = e^{-\xi}$ and $C = 1$. □

To the best of our knowledge, Theorem 6.1 is an original result.

Chapter 7

Summary and Conclusions

In this thesis, the coagulation-fragmentation equation was investigated with various coagulation kernels and constant fragmentation kernel.

Chapters 1 and 2 discussed the history, applications and derivation of the coagulation-fragmentation model.

In Chapter 3, we investigated the coagulation-fragmentation model with a constant coagulation kernel and arbitrary initial condition. The associated PDE required knowing $M_0(t)$ and $M_1(t)$ which was published in [5] and [1], respectively. An exact and explicit equation for $N_k(t)$, which until now was unknown, was determined using an inductive argument. This is the only model where an exact formula was found; but the formula has one shortcoming: before determining $N_k(t)$, the previous ones, that is, $N_1(t)$, $N_2(t)$, ..., $N_{k-1}(t)$, must first be determined. Lastly, an example for $N_k(t)$ with monodisperse initial condition was considered.

The next two chapters involved the sum ($K_{j,k} = B(j + k)$) and constant-sum ($K_{j,k} = A + B(j + k)$) coagulation-fragmentation models with arbitrary initial conditions. Each chapter began with a review of its pure coagulation counterpart, which Lu [3] established in 1987. The second section determined

	$L_{j,k}=0$	$L_{j,k}=b$
$K_{j,k}=A$	0	$-\frac{b}{2A}+\frac{1}{2}\sqrt{\frac{b^2}{A^2}+\frac{4bm}{A}}$
$K_{j,k}=B(j+k)$	0	$\dfrac{\epsilon m}{2m+\epsilon}$
$K_{j,k}=A+B(j+k)$	0	$-\dfrac{B}{A}\left(m+\dfrac{\epsilon A}{2}\right)+\sqrt{\dfrac{B^2}{A^2}\left(m+\dfrac{\epsilon A}{2}\right)^2+\epsilon Bm}$

Table 7.1: A comparison of $\lim_{t\to\infty} M_0(t)$ between the pure coagulation model and the coagulation-fragmentation model.

an implicit leading order formula of $N_k(t)$, which is an original result, for the coagulation-fragmentation model. Due to the challenges of solving the PDE, a regular perturbation expansion was applied. Another obstacle was not being able to invert $v(\xi,t)$ which resulted in only an implicit solution for $N_k(t)$. A by-product of investigating $N_k(t)$ were the previously known solutions of $M_0(t)$ [2] and $M_1(t)$ [1].

In Chapter 6, we extended the work of Brunelle et al. [5] and obtained the original result that gelation time for the pure coagulation model occurs sooner than when fragmentation is added (refer to Theorem 6.1) under a monodisperse initial condition. The pure coagulation results needed to prove Theorem 6.1 were borrowed from [25].

Since exact formulas of $M_0(t)$ are known for the constant, sum and constant-sum coagulation-fragmentation models, a comparison amongst the models and their pure coagulation versions is considered. In all three models, it is clear from Table 7.1 that under pure coagulation, $\lim_{t\to\infty} M_0(t) = 0$ while the coagulation-fragmentation model has $\lim_{t\to\infty} M_0(t) > 0$. In the continuous case, a similar observation that $M_0(t)$ approaches a positive limit was discussed in [2]. Physically, this makes sense because the presence of fragmentation counteracts the aggregation of clusters and the emptying of the system

	$L_{j,k}=0$	$L_{j,k}=b$
$K_{j,k}=A$	$\dfrac{2}{At}$	$a_1+\frac{(h_1-a_1)(a_1-a_2)}{h_1-a_2}e^{-\frac{A}{2}(a_1-a_2)t}$ where $a_1=-\frac{b}{2A}+\frac{1}{2}\sqrt{\frac{b^2}{A^2}+\frac{4bm}{A}}$ $a_2=-\frac{b}{2A}-\frac{1}{2}\sqrt{\frac{b^2}{A^2}+\frac{4bm}{A}}$
$K_{j,k}=B(j+k)$	h_0e^{-Bmt}	$\dfrac{\epsilon m}{2m+\epsilon}+(h_0-\frac{\epsilon m}{2m+\epsilon})e^{-B(m+\frac{\epsilon}{2})t}$
$K_{j,k}=A+B(j+k)$	$\frac{2h_0Bm}{2Bm+Ah_0}e^{-Bmt}$	$a_1+\frac{(h_0-a_1)(a_1-a_2)}{h_0-a_2}e^{-\frac{A}{2}(a_1-a_2)t}$ where $a_1=-\frac{B}{A}\left(m+\frac{\epsilon A}{2}\right)+\sqrt{\frac{B^2}{A^2}\left(m+\frac{\epsilon A}{2}\right)^2+\epsilon Bm}$ $a_2=-\frac{B}{A}\left(m+\frac{\epsilon A}{2}\right)-\sqrt{\frac{B^2}{A^2}\left(m+\frac{\epsilon A}{2}\right)^2+\epsilon Bm}$

Table 7.2: A comparison of the leading behaviour of $M_0(t)$ between the pure coagulation model and the coagulation-fragmentation model.

observed under pure coagulation does not occur. Also, from Table 7.2, it is clear $M_0(t)$ decays whether fragmentation is present or not but the decay is faster once fragmentation appears.

The comparison of $M_1(t)$ is simple. From [1, 16], we know any combination of $K_{j,k}=A+B(j+k)$ leads to conservation of total mass. This is true whether the fragmentation kernel is $L_{j,k}=b$ or 0. For $K_{j,k}=Cjk$, it is only known that mass is lost for the pure coagulation model [16]. However, we have established that gelation occurs sooner when fragmentation is not present.

A comparison of $N_k(t)$ is lacking. Since only the constant model resulted in an exact solution of $N_k(t)$, it does not seem prudent to establish a comparison between the models.

7.1 Future Work

In this thesis, we investigated the coagulation-fragmentation model with a bilinear kernel and a constant fragmentation kernel. But what if the fragmentation kernel was changed to a bilinear kernel? As was done in this thesis, special cases of the bilinear fragmentation kernel can be investigated. Of particular interest would be the case of both coagulation and fragmentation kernel being products. Gelation may not even occur in this situation.

It would also be desirable to find exact equations for $N_k(t)$ for the sum and constant-sum coagulation-fragmentation models. This could be achieved by modifying the generating function to form a more workable PDE or transforming (1.2) into two terms as Lu did in [3] for the pure coagulation model. Once exact solutions are known, a comparison between the constant, sum and constant-sum models for $N_k(t)$ can be investigated. Are the equations for $N_k(t)$ similar to $M_0(t)$? Do they have similar properties? Does the equation for $N_k(t)$ behave differently for k small as opposed to k large?

For the product model, Theorem 6.1 can be expanded by showing for sufficiently large ϵ, gelation is suppressed which would support the numerical results in [5]. We can also determine $N_k(t)$ and post-gelation behaviour using some of the suggestions discussed in the previous paragraph.

Bibliography

[1] J.M. Ball and J. Carr. The discrete coagulation-fragmentation equations: existence, uniqueness, and density conservation. *Journal of Statistical Physics.*, 61:203–234, 1990.

[2] John D Barrow. Coagulation with fragmentation. *J. Phys. A: Math. Gen*, 14:729–733, 1981.

[3] Lu Binglin. The exact solution of the coagulation equation with kernel $k_{ij} = a(i+j) + b$. *J. Phys. A*, 20:2347–2356, 1987.

[4] P.J. Blatz and A.V. Tobolsky. Note on the kinetics of systems manifesting simultaneous polymerization-depolymerization phenomena. *J. Phys. Chem*, 49(77-80), 1945.

[5] Eric Brunelle, Robert G. Owens, and Henry van Roessel. Gelation time in the discrete coagulation-fragmenation equations with a bilinear coagulation kernel. *Journal of Physics A: Mathematical and Theoretical*, 40(39):11749–11764, 2007.

[6] F.P. da Costa. Existence and uniquness of density conserving solutions to the coagulation-fragmentation equations with strong fragmentation. *Journal of Mathematical Analysis and Applications*, 192:892–914, 1995.

[7] R.L. Drake. *A general mathematical survey of the coagulation equation*, volume 3 of *Topics in Current Aerosol Research (Part 2)*. Pergamon Press, 1972.

[8] M.H. Ernst, R. M. Ziff, and E. M. Hendriks. Coagulation processes with a phase transition. *Journal of Colloid and Interface Science*, 97(1):266–277, 1984.

[9] M. Escobedo, Ph. Laurençot, S. Mischler, and B. Perthame. Gelation and mass conservation in coagulation-fragmentation models. *Journal of Differential Equations*, 195:143–174, 2003.

[10] M. Escobedo, S. Mischler, and B. Perthame. Gelation in coagulation and fragmentation models. *Communications in Mathematical Physics*, 231:157–188, 2002.

[11] J.B. McLeod. On an infinite set of non-linear differential equations. *Quart. J. Math. Oxford*, 13:119–125, 1962.

[12] Z. A. Melzak. A scalar transport equation. *Transactions of the American Mathematical Society*, 85(2):547–560, 1957.

[13] Fred S. Roberts and Barry Tesman. *Applied Combinatorics*. Pearson Prentice Hall, 2nd edition, 2005.

[14] R.W. Samsel and A.S. Perelson. Kinetics of rouleau formation. *Biophysical Journal*, 37(493-514), 1982.

[15] M Shirvani and J D R Stock. On mass-conserving solutions of the discrete coagulation equation. *J. Phys. A: Math. Gen.*, 21:1069–1078, 1987.

[16] M. Shirvani and H. van Roessel. The mass-conserving solutions of Smoluchowski's coagulation equation: The general bilinear kernel. *Z. Angew. Math Phys*, 43:526–535, 1992.

[17] M. Shirvani and H. van Roessel. Existence and uniquess of solutions of Smoluchowski's coagulation equation with source terms. *Quarterly of Applied Mathematics*, LX(1):183–194, 2002.

[18] J. Spouge. An existence theorem for the discrete coagulation-fragmentation equations. *Math. Proc. Camb. Phil. Soc.*, 96:183–185, 1985.

[19] John L. Spouge. Solutions and critical times for the polydisperse coagultion equation with a(x,y)=a+b(x+y)+cxy. *J. Phys. A: Math. Gen.*, 16:3127–3132, 1983.

[20] I.W. Stewart. A global existence theorem for the general coagulation-fragmentation equation with unbounded kernels. *Mathematical Methods in the Applied Sciences*, 11:627–648, 1989.

[21] I.W. Stewart. A uniqueness theorem for the coagulation-fragmentation equation. *Math. Proc. Camb. Phil. Soc.*, 107:573–578, 1990.

[22] H.J. van Roessel and M. Shirvani. A formula for the post-gelation mass of a coagultion equation with a separable bilinear kernel. *Physica D: Nonlinear Phenomena*, 222:29–36, 2006.

[23] M. von Smoluchowski. Drei Vorträgeu über Diffusion, Brownsche Bewegung und Koagulation von Kolloidteilchen. *Z. Phys.*, 17:557–585, 1916.

[24] M. von Smoluchowski. Versuch einer mathematischen Theorie der Koagulationskinetik kolloider Lösungen. *Z. Phys. Chem.*, 92:124–168, 1917.

[25] R M Ziff, M H Ernst, and E M Hendriks. Kinetics of gelation and universality. *J. Phys. A: Math. Gen*, 16:2293–2320, 1982.

[26] R.M. Ziff and G. Stell. Kinetics of polymer gelation. *The Journal of Chemical Physics*, 73:3492–3499, 1980.

Appendix A

Proof of (3.12) : Step 2 Details

$$
\begin{aligned}
&\frac{d^{k+1}}{d\xi^{k+1}}\frac{dz}{dt} + A(M_0 - \frac{\epsilon}{2})\frac{d^{k+1}z}{d\xi^{k+1}} = A\sum_{n=1}^{\frac{k-1}{2}}\binom{k}{n}\left[\frac{d^{n+1}z}{d\xi^{n+1}}\frac{d^{k-n}z}{d\xi^{k-n}} + \frac{d^{n}z}{d\xi^{n}}\frac{d^{k-n+1}z}{d\xi^{k-n+1}}\right] \\
&+ A\frac{dz}{d\xi}\frac{d^k z}{d\xi^k} + Az\frac{d^{k+1}z}{d\xi^{k+1}} + b\Bigg[\frac{d^{k+1}z}{d\xi^{k+1}}\frac{1}{\xi e^{\frac{bt}{2}} - 1} - \frac{d^k z}{d\xi^k}\frac{e^{\frac{bt}{2}}}{(\xi e^{\frac{bt}{2}} - 1)^2} \\
&+ \sum_{n=2}^{k-1}\frac{k!}{n!}\left[\frac{(-1)^{k-n}\frac{d^{n+1}z}{d\xi^{n+1}}e^{\frac{(k-n)bt}{2}}}{(\xi e^{\frac{bt}{2}} - 1)^{k+1-n}} - \frac{\frac{d^n z}{d\xi^n}e^{\frac{(k-n+1)bt}{2}}(k+1-n)}{(\xi e^{\frac{bt}{2}} - 1)^{k+2-n}}\right] \\
&+ (-1)^{k+1}k!\frac{d^2 z}{d\xi^2}\frac{e^{\frac{(k-1)bt}{2}}}{(\xi e^{\frac{bt}{2}} - 1)^k} - \frac{(-1)^{k+1}k!\left(\frac{dz}{d\xi} - M_0 e^{\frac{bt}{2}}\right)e^{\frac{kbt}{2}}k}{(\xi e^{\frac{bt}{2}} - 1)^{k+1}} \\
&+ \frac{(-1)^k k!\left(\frac{dz}{d\xi} - M_0 e^{\frac{bt}{2}}\right)e^{\frac{kbt}{2}}}{(\xi e^{\frac{bt}{2}} - 1)^{k+1}} - \frac{(k+1)(-1)^k k!\left[z - M_0\xi e^{\frac{bt}{2}}\right]e^{\frac{(k+1)bt}{2}}}{(\xi e^{\frac{bt}{2}} - 1)^{k+2}}\Bigg].
\end{aligned}
$$

Applying the combinatorics' identity

$$\binom{k}{n} = \binom{k+1}{n} - \binom{k}{n-1}$$

and combining the $3rd$ and $2nd$ last terms,

$$\frac{d^{k+1}}{d\xi^{k+1}}\frac{dz}{dt} + A(M_0 - \frac{\epsilon}{2})\frac{d^{k+1}z}{d\xi^{k+1}} = A\sum_{n=1}^{\frac{k-1}{2}}\binom{k+1}{n}\frac{d^n z}{d\xi^n}\frac{d^{k-n+1}z}{d\xi^{k-n+1}}$$

$$+ A\sum_{n=1}^{\frac{k-1}{2}}\binom{k}{n}\frac{d^n z}{d\xi^n}\frac{d^{k-n}z}{d\xi^{k-n}} - A\sum_{n=1}^{\frac{k-1}{2}}\binom{k}{n-1}\frac{d^n z}{d\xi^n}\frac{d^{k-n+1}z}{d\xi^{k-n+1}} + A\frac{dz}{d\xi}\frac{d^k z}{d\xi^k} + Az\frac{d^{k+1}z}{d\xi^{k+1}}$$

$$+ b\left[\frac{d^{k+1}z}{d\xi^{k+1}}\frac{1}{\xi e^{\frac{bt}{2}} - 1} - \frac{d^k z}{d\xi^k}\frac{e^{\frac{bt}{2}}}{(\xi e^{\frac{bt}{2}} - 1)^2} + \sum_{n=2}^{k-1}\frac{k!}{n!}\frac{(-1)^{k-n}\frac{d^{n+1}z}{d\xi^{n+1}}e^{\frac{(k-n)bt}{2}}}{(\xi e^{\frac{bt}{2}} - 1)^{k+1-n}}\right.$$

$$+ \sum_{n=2}^{k-1}\frac{k!}{n!}\frac{(-1)^{k-n}\frac{d^n z}{d\xi^n}e^{\frac{(k+1-n)bt}{2}}(k+1-n)}{(\xi e^{\frac{bt}{2}} - 1)^{k+2-n}} + (-1)^{k+1}k!\frac{d^2 z}{d\xi^2}\frac{e^{\frac{(k-1)bt}{2}}}{(\xi e^{\frac{bt}{2}} - 1)^k}$$

$$\left. + \frac{(-1)^{(k+2)}(k+1)!\left(\frac{dz}{d\xi} - M_0 e^{\frac{bt}{2}}\right)e^{\frac{kbt}{2}}}{(\xi e^{\frac{bt}{2}} - 1)^{k+1}} - \frac{(k+1)!(-1)^k\left(z - M_0\xi e^{\frac{bt}{2}}\right)e^{\frac{(k+1)bt}{2}}}{(\xi e^{\frac{bt}{2}} - 1)^{k+2}}\right].$$

After merging the third sum with $A\frac{dz}{d\xi}\frac{d^k z}{d\xi^k}$, then relabelling it with $m = n - 1$ and subtracting from the second sum,

$$\frac{d^{k+1}}{d\xi^{k+1}}\frac{dz}{dt} + A(M_0 - \frac{\epsilon}{2})\frac{d^{k+1}z}{d\xi^{k+1}} = A\sum_{n=1}^{\frac{k-1}{2}}\binom{k+1}{n}\frac{d^n z}{d\xi^n}\frac{d^{k-n+1}z}{d\xi^{k-n+1}}$$

$$+ A\binom{k}{\frac{k+1}{2}}\left(\frac{d^{\frac{k+1}{2}}z}{d\xi^{\frac{k+1}{2}}}\right)^2 + Az\frac{d^{k+1}z}{d\xi^{k+1}} + b\left[\frac{d^{k+1}z}{d\xi^{k+1}}\frac{1}{\xi e^{\frac{bt}{2}} - 1}\right.$$

$$- \frac{d^k z}{d\xi^k}\frac{e^{\frac{bt}{2}}}{(\xi e^{\frac{bt}{2}} - 1)^2} + \sum_{n=2}^{k-1}\frac{k!}{n!}\frac{(-1)^{k-n}\frac{d^{n+1}z}{d\xi^{n+1}}e^{\frac{(k-n)bt}{2}}}{(\xi e^{\frac{bt}{2}} - 1)^{k+1-n}}$$

$$+ \sum_{n=2}^{k-1}\frac{k!}{n!}\frac{(-1)^{k-n}\frac{d^n z}{d\xi^n}e^{\frac{(k+1-n)bt}{2}}(k+1-n)}{(\xi e^{\frac{bt}{2}} - 1)^{k+2-n}} + (-1)^{k+1}k!\frac{d^2 z}{d\xi^2}\frac{e^{\frac{(k-1)bt}{2}}}{(\xi e^{\frac{bt}{2}} - 1)^k}$$

$$\left. + \frac{(-1)^{(k+2)}(k+1)!\left(\frac{dz}{d\xi} - M_0 e^{\frac{bt}{2}}\right)e^{\frac{kbt}{2}}}{(\xi e^{\frac{bt}{2}} - 1)^{k+1}} - \frac{(k+1)!(-1)^k\left(z - M_0\xi e^{\frac{bt}{2}}\right)e^{\frac{(k+1)bt}{2}}}{(\xi e^{\frac{bt}{2}} - 1)^{k+2}}\right].$$

Coupling the $2nd$ and $3rd$ sum with $(-1)^{k+1}k!\frac{d^2z}{d\xi^2}\frac{e^{\frac{(k-1)bt}{2}}}{(\xi e^{\frac{bt}{2}}-1)^k}$ and $-\frac{d^k z}{d\xi^k}\frac{e^{\frac{bt}{2}}}{(\xi e^{\frac{bt}{2}}-1)^2}$ respectively,

$$\frac{d^{k+1}}{d\xi^{k+1}}\frac{dz}{dt} + A(M_0 - \frac{\epsilon}{2})\frac{d^{k+1}z}{d\xi^{k+1}} = A\sum_{n=1}^{\frac{k-1}{2}}\binom{k+1}{n}\frac{d^n z}{d\xi^n}\frac{d^{k-n+1}z}{d\xi^{k-n+1}}$$
$$+ A\binom{k}{\frac{k+1}{2}}\left(\frac{d^{\frac{k+1}{2}}z}{d\xi^{\frac{k+1}{2}}}\right)^2 + Az\frac{d^{k+1}z}{d\xi^{k+1}} + b\Bigg[\frac{d^{k+1}z}{d\xi^{k+1}}\frac{1}{\xi e^{\frac{bt}{2}} - 1}$$
$$+ \sum_{n=2}^{k}\frac{k!}{n!}\frac{(-1)^{k-n}\frac{d^n z}{d\xi^n}e^{\frac{(k-n+1)bt}{2}}(k+1-n)}{(\xi e^{\frac{bt}{2}} - 1)^{k+2-n}}$$
$$+ \sum_{n=1}^{k-1}\frac{k!}{n!}\frac{(-1)^{k-n}\frac{d^{n+1}z}{d\xi^{n+1}}e^{\frac{(k-n)bt}{2}}}{(\xi e^{\frac{bt}{2}} - 1)^{k+1-n}} + \frac{(-1)^{(k+2)}(k+1)!\left(\frac{dz}{d\xi} - M_0 e^{\frac{bt}{2}}\right)e^{\frac{kbt}{2}}}{(\xi e^{\frac{bt}{2}} - 1)^{k+1}}$$
$$- \frac{(k+1)!(-1)^k\left(z - M_0\xi e^{\frac{bt}{2}}\right)e^{\frac{(k+1)bt}{2}}}{(\xi e^{\frac{bt}{2}} - 1)^{k+2}}\Bigg].$$

Finally, by relabelling the $3rd$ sum with $n = m - 1$ and uniting with the $2nd$ sum,

$$\frac{d^{k+1}}{d\xi^{k+1}}\frac{dz}{dt} + A(M - \frac{\epsilon}{2})\frac{d^{k+1}z}{d\xi^{k+1}} = A\sum_{n=1}^{\frac{k-1}{2}}\binom{k+1}{n}\frac{d^n z}{d\xi^n}\frac{d^{k+1-n}z}{d\xi^{k+1-n}} + A\binom{k}{\frac{k+1}{2}}\left(\frac{d^{\frac{k+1}{2}}z}{d\xi^{\frac{k+1}{2}}}\right)^2$$
$$+ Az\frac{d^{k+1}z}{d\xi^{k+1}} + b\Bigg[\frac{d^{k+1}z}{d\xi^{k+1}}\frac{1}{\xi e^{\frac{bt}{2}} - 1} + \sum_{n=2}^{k}\frac{(-1)^{k+1-n}\frac{(k+1)!}{n!}\frac{d^n z}{d\xi^n}e^{\frac{(k+1-n)bt}{2}}}{(\xi e^{\frac{bt}{2}} - 1)^{k-n+2}}$$
$$+ \frac{(-1)^{k+2}(k+1)!(\frac{dz}{d\xi} - M_0 e^{\frac{bt}{2}})e^{\frac{kbt}{2}}}{(\xi e^{\frac{bt}{2}} - 1)^{k+1}} + \frac{(-1)^{k+1}(k+1)!(z - M_0\xi e^{\frac{bt}{2}})e^{\frac{(k+1)bt}{2}}}{(\xi e^{\frac{bt}{2}} - 1)^{k+2}}\Bigg]$$

as desired.

Appendix B

Detailed Proof of (3.16)

We now prove the integrals of (3.16) exist.

Proof: (by strong induction)

Step 1: Show the $j = 2$ case is true.

In other words, show

$$f_2(t)\mu(t) - f_0'(a_1 - a_2)^2 = A\int_0^t f_1^2 \mu d\bar{t} - 2b\int_0^t f_1 e^{\frac{b\bar{t}}{2}}\mu d\bar{t} + 2b\int_0^t M_0 e^{b\bar{t}}\mu d\bar{t}$$

exists. The middle and last terms can be explicitly solved. The first term cannot be explicitly determined but can be shown to exist by proving the integrand, $f_1^2\mu$, is continuous. To prove continuity of

$$f_1^2\mu = \frac{\left[f_{10}(a_1 - a_2)^2 + 2\epsilon(h_1 - a_1)(h_1 - a_2)(e^{\frac{bt}{2}} - 1) - \epsilon\frac{a_1}{a_2}(h_1 - a_2)^2(e^{-Aa_2t} - 1) + \epsilon\frac{a_2}{a_1}(h_1 - a_1)^2(e^{-Aa_1t} - 1)\right]^2}{(h_1 - a_2 - (h_1 - a_1)e^{\frac{-A(a_1-a_2)t}{2}})^2 e^{\frac{A(a_1-a_2)t}{2}}},$$

we must show its denominator$\neq 0$ for all $t \in [0, \infty)$.

Prove $(h_1 - a_2 - (h_1 - a_1)e^{\frac{-A(a_1-a_2)t}{2}})^2 e^{\frac{A(a_1-a_2)t}{2}} \neq 0$. for all $t \in [0, \infty)$

Proof: (by contradiction)

Suppose there exists for some $\bar{t} \in [0, \infty)$ such that

$$(h_1 - a_2 - (h_1 - a_1)e^{\frac{-A(a_1-a_2)\bar{t}}{2}})^2 e^{\frac{A(a_1-a_2)\bar{t}}{2}} = 0$$

$$\Leftrightarrow \quad \frac{h_1 - a_2}{h_1 - a_1} = e^{-\frac{A(a_1-a_2)\bar{t}}{2}}$$

$$\Leftrightarrow \quad \bar{t} = \frac{-2}{A(a_1 - a_2)} \ln\left(\frac{h_1 - a_2}{h_1 - a_1}\right)$$

$$\Leftrightarrow \quad \ln\left(\frac{h_1 - a_2}{h_1 - a_1}\right) \leq 0 \text{ would satisfy the assumption since } \frac{-2}{A(a_1 - a_2)} < 0$$

$$\Leftrightarrow \quad 0 < \frac{h_1 - a_2}{h_1 - a_1} \leq 1.$$

But (3.7) and (3.8) $\Rightarrow a_1 > a_2 \Rightarrow h_1 - a_1 > h_1 - a_2 \Rightarrow \frac{h_1 - a_1}{h_1 - a_2} > 1$ which contradicts the assumption. Therefore, $f_1^2\mu$ is continuous, which means $\int_0^t f_1^2 \mu d\bar{t}$ exists. It has now been shown case $j = 2$ is true.

Step 2: Assume the $j = 1, 2, .., k$ cases are true.
(i.e. assume the integrals of (3.16) all exist).

Step 3: Show the $k + 1$ case is true.
Without lose of generality, assume k is even $\Rightarrow k + 1$ is odd. We have to show the following integrals:

$$\int_0^t f_n f_{k+1-n} \mu d\bar{t}, \quad \int_0^t f_n e^{\frac{(k+1-n)b\bar{t}}{2}} \mu d\bar{t}, \quad \text{and} \quad \int_0^t [f_1(t) - M_0(t)e^{\frac{b\bar{t}}{2}}] e^{\frac{kb\bar{t}}{2}} \mu d\bar{t}$$

all exist. The last integral can be solved explicitly by substituting in (3.15) and (3.9). To show the first integral exists will require a bit more work. First, assume n and $k + 1 - n$ are both odd. (All the different even and odd combinations can be shown in an identical manner.) Since $n \leq k$ and $k + 1 - n \leq k$ for all $n = 1, ..., \frac{k-1}{2}$, replace $f_n f_{k+1-n}$ with (3.16) which, by the assumption in step 2, exists. Since (3.16) exists, then it must also be continuous. Therefore,

$$\int_0^t f_n f_{k+1-n}\mu d\bar{t} = \int_0^t \left[\frac{f_{n0}(a_1-a_2)^2}{\mu} + \frac{A}{\mu}\sum_{i=1}^{\frac{n-1}{2}} \binom{n}{i} \int_0^{\bar{t}} f_i f_{n-i}\mu dr \right.$$

$$\left. - \frac{b}{\mu}\sum_{i=2}^{n-1}\frac{n!}{i!}\int_0^{\bar{t}} f_i e^{\frac{(n-i)br}{2}}\mu dr - \frac{bn!}{\mu}\int_0^{\bar{t}}[f_1(r) - M_0(r)e^{\frac{br}{2}}]e^{\frac{(n-1)br}{2}}\mu dr \right] *$$

$$\left[f_{(k+1-n)0}(a_1-a_2)^2 + A\sum_{i=1}^{\frac{k-n}{2}} \binom{n}{i} \int_0^{\bar{t}} f_i f_{k+1-n-i}\mu dr \right.$$

$$- b\sum_{i=2}^{k-n}\frac{(k+1-n)!}{i!}\int_0^{\bar{t}} f_i e^{\frac{(k+1-n-i)br}{2}}\mu dr$$

$$\left. -b(k+1-n)!\int_0^{\bar{t}}[f_1(r) - M_0(r)e^{\frac{br}{2}}]e^{\frac{(k-n)br}{2}}dr \right] d\bar{t}$$

exists. The existence of the second integral is achieved in the same fashion. Therefore, by the principle of mathematical induction, (3.16) is true. □