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COAGULATION AND FRAGMENTATION PROCESSES WITH EVOLVING SIZE AND SHAPE PROFILES: A SEMIGROUP APPROACH

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Abstract. We investigate a class of bivariate coagulation-fragmentation equations. These equations describe the evolution of a system of particles that are characterised not only by a discrete size variable but also by a shape variable which can be either discrete or continuous. Existence and uniqueness of strong solutions to the associated abstract Cauchy problems are established by using the theory of substochastic semigroups of operators.

1. **Introduction.** When modelling coagulation-fragmentation (C-F) processes, an assumption which is usually made is that the particles, or clusters, in the evolving system can be distinguished by means of a single size variable, such as mass. The resulting model describing the continuous time evolution of the system then takes the form of either an integro-differential equation, when the size variable is permitted to take any positive value, or an infinite system of ordinary differential equations (ODEs) when the mass of a cluster is always an integer multiple of some fundamental unit (the mass of an atom or monomer).

Many mathematical investigations into both continuous-size integro-differential models and discrete-size ODE models have been conducted with the aim of resolving questions such as well-posedness and long-term behaviour of solutions. In particular, in two recent papers [9, 10], we considered a system of particles with evolving discrete sizes, and by studying appropriate abstract Cauchy problems (ACPs), we obtained existence and uniqueness results for strong solutions by applying the theory of substochastic semigroups of operators; see [1, Chapter 6]. Prior to these papers, only continuous models of C–F processes had been studied via semigroup-based techniques. In the case of discrete models, the favoured method had invariably involved analysing truncated versions of the infinite set of ODEs and then showing

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To Jerry Goldstein on his 70^{th} birthday with all good wishes for the future.

that, from the solutions of the resulting finite-dimensional systems, a subsequence could be extracted which converged to an appropriately defined solution [4, 5]. The results we established via semigroups in [9] have since been extended by Banasiak [2] who used properties of analytic semigroups to relax some of the conditions required in [9].

Clearly, single-component C-F models of the type described above fail to give an adequate description of processes in which cluster shape is not preserved under coalescence or break-up. Processes of this type can arise, for example, in dust aggregation where two dust aggregates can collide to form a single aggregate which, due to a restructuring mechanism, has a different morphology to the constituent aggregates [3]. Motivated by this, a number of multi-component C-F models have been proposed and investigated; see [6, 7, 8, 12, 13] and the references contained therein.

As far as we are aware, the question of existence and uniqueness of solutions to a general class of multi-component C-F equations has yet to be addressed. Consequently, in this paper we shall demonstrate that the semigroup approach used for single-component equations can be adapted to cater for bivariate models of the type suggested by Wattis in [13]. Therefore, we shall investigate a system in which not only the cluster size can change but also the shape profile can evolve.

Clearly, there is no unique way of describing the shape of a cluster, and the choice of appropriate variables used in any multi-component model to distinguish between two clusters of the same size but different morphologies will depend on the nature of the underlying physical system. In this paper, we shall assume that particles join together in a lattice formation and shall initially represent the 'shape' of a cluster by means of a single discrete variable which we shall refer to as the 'diameter' of the cluster. For example, the value of this 'diameter' variable could be taken to be the maximal extension in a direction of a coordinate axis. In this case, for a cluster composed of n particles, the maximum possible diameter is n, whilst the minimum possible diameter is $d_{min2D}(n) = \lceil \sqrt{n} \rceil$ in two dimensions, and $d_{min3D}(n) = \lceil \sqrt[3]{n} \rceil$ in three dimensions, where $\lceil x \rceil$ represents the smallest integer $\geq x$. It is important to note, however, that the analytical approach we use here is flexible enough to cater for other interpretations of the diameter of a cluster of particles, and, to highlight this fact, we consider a 'mixed' model in Section 4 in which the size of a cluster is still represented by a discrete variable, but the 'diameter' is a continuous variable.

We let $u_{n,j}$ denote the concentration of clusters of mass n and diameter j. As mentioned above, we assume that clusters take the form of lattices, with

- the minimum diameter of a cluster of mass n denoted by $d_{min}(n) \geq 1$; (1)
- the maximum diameter of a cluster of mass n given by n so that

$$u_{n,j} = 0 \text{ for } j > n. \tag{2}$$

In addition, we make the assumption that the mass and diameter in any coagulation event are additive so that

$$u_{n,j} + u_{r,s} \to u_{n+r,j+s}\,. \tag{3}$$

Mass additivity is assumed in many models in the literature. However, it is apparent that a coagulation event involving clusters of diameters j and s may result in a cluster of diameter l which is smaller than $j + s$. As in [13, p.7285], we are using the fact that our model incorporates a restructuring mechanism to reduce the

diameter of a cluster to provide some justification for considering only the 'worst' case scenario of the greatest possible value for l. It should also be noted that the model we discuss here can be extended to one which allows for the formation of clusters with diameters less than the maximum; we shall comment further on this later in the paper.

The coagulation-reformation equations derived by Wattis [13, eqn. (2.2)] take the form

$$\begin{aligned}
\frac{du_{n,n}}{dt} &= F_{n,n} - L_{n,n} - \gamma_{n,n}u_{n,n}, \\
\frac{du_{n,j}}{dt} &= F_{n,j} - L_{n,j} + \gamma_{n,j+1}u_{n,j+1} - \gamma_{n,j}u_{n,j}, \qquad d_{min}(n)+1 \le j < n \\
\frac{du_{n,j}}{dt} &= F_{n,j} - L_{n,j} + \gamma_{n,j+1}u_{n,j+1}, \qquad j = d_{min}(n) < n
\end{aligned} \tag{4}$$

where $n = 1, 2, \ldots$, and

$$F_{n,j} = \frac{1}{2}\sum_{r=1}^{n-1}\sum_{s=1}^{j-1} k_{n-r,r,j-s,s}u_{n-r,j-s}u_{r,s} \tag{5}$$

is the gain in clusters of mass n, diameter j due to the coagulation of clusters $u_{r,s}$ and $u_{n-r,j-s}$. Note that $F_{n,j} = 0$ for $n = 1$ or $j = 1$ since there cannot be a gain in clusters of mass one or diameter one due to a coagulation event. Similarly

$$L_{n,j} = \sum_{r=1}^{\infty}\sum_{s=1}^{\infty} k_{n,r,j,s}u_{n,j}u_{r,s} \tag{6}$$

is the loss of clusters of mass n, diameter j due to the coagulation of clusters $u_{n,j}$ and $u_{r,s}$. The coefficient $k_{r,n,s,j}$ represents the rate of coagulation of clusters $u_{r,s}$ and $u_{n,j}$. The reformation coefficient $\gamma_{n,j}$ gives the rate at which a cluster $u_{n,j}$ will reshape to create a cluster with smaller diameter, $u_{n,j-1}$. As in [13], we shall set $d_{min}(n) = 1$ for each n, in which case, in addition to (2), for the model to make physical sense we must have

$$\gamma_{n,1} = 0 \qquad \text{for } n = 1, 2, \ldots. \tag{7}$$

Then the three equations in (4) can be combined to give

$$\frac{du_{n,j}}{dt} = F_{n,j} - L_{n,j} + \gamma_{n,j+1}u_{n,j+1} - \gamma_{n,j}u_{n,j} \quad (1 \le j \le n). \tag{8}$$

In [13], attention is focussed on the specific case when the coagulation rate coefficients $k_{n,r,j,s}$ are independent of size and shape; in addition, the reformation coefficients $\gamma_{n,j}$ are independent of n and are given by $\gamma_{n,j} = \gamma(j-1)$, with γ constant. Moreover, it is assumed in [13] that $d_{min}(n) = 1$ for all n and that, initially, the system is completely in monomeric form, that is, the initial data are $u_{n,j} = 0$ for all n, j, with the exception of $u_{1,1} = \rho$, for some constant ρ. These assumptions are not required for the results that we obtain here. Not only can we cater for a class of initial conditions, and place less restrictive assumptions on the coagulation and reformation rate terms, we shall also consider a more general version of (8) in which *any* cluster with diameter greater than j (and not just of diameter $j+1$) can reform to produce a cluster with diameter j. For this we replace the third term,

$\gamma_{n,j+1}u_{n,j+1}$, in (8) by

$$\sum_{s=j+1}^{n} \gamma_{n,s}p_{n,j,s}u_{n,s} \tag{9}$$

where $\gamma_{n,s}$ is the reformation rate of a cluster with mass n, diameter s and $p_{n,j,s}$ is the probability that a cluster with mass n, diameter s will reform to produce a cluster with mass n, diameter j. Note that again we have $u_{n,j} = 0$ for $j > n$. Naturally, since $p_{n,j,s}$ is a probability, we require

$$\sum_{j=1}^{s-1} p_{n,j,s} = 1, \qquad 0 \leq p_{n,j,s} \leq 1. \tag{10}$$

Note that $p_{n,j,j} = 0$ since we assume that a reformation event always changes the diameter of a cluster. Also, for physical reasons we require $p_{n,j,s} = 0$ if $j > n$ or $s > n$. For each $n = 1, 2, \ldots$ and $j \leq n$ the evolution of clusters of mass n and diameter j is then described by

$$\frac{du_{n,j}(t)}{dt} = F_{n,j} - L_{n,j} + \sum_{s=j+1}^{\infty} \gamma_{n,s}p_{n,j,s}u_{n,s}(t) - \gamma_{n,j}u_{n,j}(t). \tag{11}$$

Note that (8) can be obtained from (11) by choosing $p_{n,j,s} = 1$ when $s = j+1$ and $p_{n,j,s} = 0$ otherwise.

The appropriate space in which to formulate the corresponding ACP is defined as follows.

Definition 1.1. Let X denote the vector space of all real doubly infinite sequences $f = \{f_{n,j}\}_{n,j=1}^{\infty}$ such that

$$\begin{gathered} f_{n,j} = 0 \text{ for } j > n, \\ \|f\| := \sum_{n=1}^{\infty}\sum_{j=1}^{\infty} n|f_{n,j}| = \sum_{n=1}^{\infty}\sum_{j=1}^{n} n|f_{n,j}| < \infty. \end{gathered} \tag{12}$$

Remark 1. It can be shown fairly easily that $(X, \|\cdot\|)$ is a Banach space.

2. The Reformation Semigroup.

We begin by considering only the reformation terms in (11), i.e.

$$\frac{du_{n,j}(t)}{dt} = \sum_{s=j+1}^{\infty} \gamma_{n,s}p_{n,j,s}u_{n,s}(t) - \gamma_{n,j}u_{n,j}(t) \quad (1 \leq j \leq n). \tag{13}$$

The corresponding ACP requires a function $u : [0, \infty) \to X$ to be found such that

$$\frac{d}{dt}u(t) = Au(t) + Bu(t) \quad (t > 0), \qquad \lim_{t\to 0+} u(t) = f \in D(A) \tag{14}$$

where

$$[Af]_{n,j} := -\gamma_{n,j}f_{n,j} = -\gamma_{n,j}f_{n,j}, \quad [Bf]_{n,j} := \sum_{s=j+1}^{\infty} \gamma_{n,s}p_{n,j,s}f_{n,s}, \tag{15}$$

with

$$\begin{aligned} D(A) &:= \{f \in X : \sum_{n=1}^{\infty}\sum_{j=1}^{n} n\gamma_{n,j}|f_{n,j}| < \infty\}; \\ D(B) &:= \{f \in X : \sum_{n=1}^{\infty}\sum_{j=1}^{n} n\Big|\sum_{s=j+1}^{\infty}\gamma_{n,s}p_{n,j,s}f_{n,s}\Big| < \infty\}. \end{aligned} \tag{16}$$

We begin by proving

Lemma 2.1. *As sets $D(A) \subseteq D(B)$.*

Proof. For $f \in D(A)$

$$\begin{aligned} \|Bf\| &\leq \sum_{n=1}^{\infty}\sum_{j=1}^{\infty} n \sum_{s=j+1}^{\infty}\gamma_{n,s}p_{n,j,s}|f_{n,s}| \\ &= \sum_{n=1}^{\infty}\sum_{s=2}^{\infty}\sum_{j=1}^{s-1} n\gamma_{n,s}p_{n,j,s}|f_{n,s}| \\ &= \sum_{n=1}^{\infty}\sum_{s=2}^{\infty} n\gamma_{n,s}|f_{n,s}| \quad \text{on using (10)} \\ &= \|Af\| \quad \text{on using (7)} \\ &< \infty. \end{aligned}$$

Hence $D(A) \subseteq D(B)$. □

Our first main result is

Theorem 2.2. *Let X, A and B be as in Definition 1.1, (15) and (16). Then there exists a smallest extension G of $A + B$ which generates a substochastic semigroup $\{T_G(t)\}_{t\geq 0}$ on X.*

Proof. We shall apply the Kato-Voigt Theorem [1, Corollary 5.17]. Firstly, we note that X is a subspace of $L^1(\Omega, \mu)$ where $\Omega = \mathbb{N} \times \mathbb{N}$ and the measure μ is defined on subsets $\mathbb{M}$ of $\mathbb{N} \times \mathbb{N}$ by

$$\mu(\mathbb{M}) = \begin{cases} \sum\limits_{(n,j)\in\mathbb{M}} n & \text{if } \mathbb{M} \subseteq \mathbb{N} \times \mathbb{N} \text{ is finite} \\ \infty & \text{if } \mathbb{M} \text{ is infinite.} \end{cases} \tag{17}$$

Under the conditions on $\gamma_{n,j}$, it is easy to check that A generates a substochastic semigroup $\{T_A(t)\}_{t\geq 0}$ on X, given by

$$[T_A(t)f]_{n,j} = \exp(-\gamma_{n,j}t)\, f_{n,j} \quad \forall\, n, j. \tag{18}$$

As shown in Lemma 2.1, $D(A) \subseteq D(B)$ and it is clear that $[Bf]_{n,j} \geq 0$ for all $f \in D(B)^+$ (the set of non-negative elements of $D(B)$). Also, from the calculations used in the proof of Lemma 2.1 we have, for $f \in D(A)^+$,

$$\int_{\Omega}(Af + Bf)d\mu = 0.$$

The result follows from the Kato-Voigt Theorem. □

We can now go on to prove the following

Theorem 2.3. *In the context of Theorem 2.2, $G = \overline{A+B}$, where $\overline{A+B}$ denotes the closure of the operator $(A+B, D(A))$.*

Proof. We shall use [1, Theorem 6.22] to which the reader should refer for the necessary notation. In our case,

$$F = \left\{ f = \{f_{n,j}\} : f_{n,j} = 0 \text{ for } j > n \text{ and } \left\{ \frac{f_{n,j}}{1+\gamma_{n,j}} \right\} \in X \right\}$$

$$[\mathbb{L}f]_{n,j} = \frac{f_{n,j}}{1+\gamma_{n,j}}, \quad f \in F;$$

$$[\mathbb{A}f]_{n,j} = -\gamma_{n,j} f_{n,j},$$

$$D(\mathbb{A}) = \mathbb{L}F = \{ f \in X : f_{n,j} = \frac{g_{n,j}}{1+\gamma_{n,j}},\ g \in F \};$$

$$[\mathbb{B}f]_{n,j} = \sum_{s=j+1}^{\infty} \gamma_{n,s} p_{n,j,s} f_{n,s},$$

$$D(\mathbb{B}) = \Bigg\{ f \in X : \text{ if } \{f^n\} \text{ is any non-negative, non-decreasing sequence in } D(B)$$
$$\text{satisfying } \sup_n f^n_{m,j} = |f_{m,j}|\ \forall m, j, \text{ then } \sup_n B f^n_{m,j} < \infty\ \forall m, j \Bigg\}.$$

We need to prove that if $g \in F^+$ is such that $-g + \mathbb{B}\mathbb{L}g \in X$ then we also have

$$\sum_{n=1}^{\infty}\sum_{j=1}^{\infty} n(\mathbb{L}g)_{n,j} + \sum_{n=1}^{\infty}\sum_{j=1}^{\infty} n\left(-g_{n,j} + (\mathbb{B}\mathbb{L}g)_{n,j}\right) \geq 0. \tag{19}$$

Let $f_{n,j} = (\mathbb{L}g)_{n,j} = (1+\gamma_{n,j})^{-1} g_{n,j}$ so that $f \in X^+$. Then equation (19) holds if, for any $f \in X^+$ such that $\mathbb{A}f + \mathbb{B}f \in X$, we have

$$\sum_{n=1}^{\infty}\sum_{j=1}^{\infty} n\left(-\gamma_{n,j} f_{n,j} + (\mathbb{B}f)_{n,j}\right) \geq 0 \tag{20}$$

since

$$(\mathbb{L}g)_{n,j} - g_{n,j} = -\frac{\gamma_{n,j}}{1+\gamma_{n,j}} g_{n,j} = -\gamma_{n,j} f_{n,j}.$$

Now (20) can be written as

$$\lim_{N\to\infty} \left(-\sum_{n=1}^{N}\sum_{j=1}^{n} n\gamma_{n,j} f_{n,j} + \sum_{n=1}^{N}\sum_{j=1}^{n} n \sum_{s=j+1}^{\infty} \gamma_{n,s} p_{n,j,s} f_{n,s} \right). \tag{21}$$

On using (10), (7) and the fact that $f_{n,s} = 0$ for $s > n$, we obtain

$$\sum_{n=1}^{N}\sum_{j=1}^{n} n \sum_{s=j+1}^{\infty} \gamma_{n,s} p_{n,j,s} f_{n,s} = \sum_{n=1}^{N}\sum_{s=2}^{\infty}\sum_{j=1}^{s-1} n\gamma_{n,s} p_{n,j,s} f_{n,s} = \sum_{n=1}^{N}\sum_{s=1}^{n} n\gamma_{n,s} f_{n,s}.$$

Thus the limit in (21) is 0, showing that the conditions of [1, Theorem 6.22] are satisfied and we can conclude that $G = \overline{A+B}$.

□

Remark 2. We can say that the semigroup $\{T_G(t)\}_{t\geq 0}$ generated by G is stochastic since, by the calculations in the proof of Lemma 2.1, $\int_\Omega (Af + Bf) d\mu = 0$.

3. **Coagulation with Reformation.** By Theorem 2.3 and Remark 2, we can deduce that the ACP

$$\frac{du(t)}{dt} = Gu(t), \;\; t > 0, \qquad \lim_{t\to 0^+} u(t) = f$$

has a unique strict, non-negative and mass-conserving solution $u : [0,\infty) \to D(G)^+$ for each $f \in D(G)^+$ and hence for each $f \in D(A)^+$. This solution is given by $u(t) = T_G(t)f$, with $G = \overline{A+B}$. We now apply a technique used in [9, Section 4] to analyse the combined coagulation-reformation equation (11). The nonlinear ACP which we wish to solve takes the form

$$\frac{d}{dt}u(t) = Gu(t) + Ku(t) \quad (t > 0), \qquad \lim_{t\to 0+} u(t) = f \in D(G)^+ \tag{22}$$

where the coagulation operator K is given by

$$[Kf]_{n,j} = \frac{1}{2}\sum_{r=1}^{n-1}\sum_{s=1}^{j-1} k_{n-r,r,j-s,s} f_{n-r,j-s} f_{r,s} - \sum_{r=1}^{\infty}\sum_{s=1}^{\infty} k_{n,r,j,s} f_{n,j} f_{r,s}. \tag{23}$$

We can show that

$$\sum_{n=1}^{\infty}\sum_{j=1}^{\infty} n[Kf]_{n,j} = 0$$

by calculations similar to those in [9, Theorem 4.8]. We shall assume that

$$k_{n,r,j,s} = k_{r,n,s,j} \tag{24}$$

and there exists a constant k such that

$$k_{n,r,j,s} \le k \quad \text{for all } n, r = 1, 2, \dots \text{ and } j \le n, s \le r. \tag{25}$$

Definition 3.1. We define $\tilde{K}$ on $X \times X$ by

$$\left(\tilde{K}[f,g]\right)_{n,j} = \frac{1}{2}\sum_{r=1}^{n-1}\sum_{s=1}^{j-1} k_{n-r,r,j-s,s} f_{n-r,j-s} g_{r,s} - \sum_{r=1}^{\infty}\sum_{s=1}^{\infty} k_{n,r,j,s} f_{n,j} g_{r,s} \tag{26}$$

with $f, g \in X$.

Theorem 3.2. *Under condition (25), $\tilde{K}$ defined in (26) is a bilinear, continuous form mapping $X \times X$ into X, with*

$$\|\tilde{K}[f,g]\| \le 2k \|f\| \|g\| \;\; \forall\, f, g \in X. \tag{27}$$

Proof. This is similar to that of [9, Theorem 4.2] □

The bound (27) is similar to that in [9, formula (4.8)]. We can then proceed to prove analogues of the other results in [9, Section 4]. We shall omit the details and simply state the final outcome.

Theorem 3.3. *There exists a global, strong, non-negative, mass-conserving solution to the ACP*

$$\frac{d}{dt}u(t) = Gu(t) + Ku(t) \quad (t \ge 0), \qquad \lim_{t\to 0+} u(t) = f \in D(G)^+$$

where $G = \overline{A+B}$.

Proof. See the preamble. □

4. **Further Generalisations.** The methods used in the previous sections can also cater for more general situations, including cases where we have a continuous shape variable and where fragmentation of clusters can also occur. To conclude, we shall outline three such generalisations. For brevity, only the salient points will be included; further details can be found in [11, Chapter 5].

4.1. **Reformation with Fragmentation.** We begin by considering the effects of fragmentation being introduced into the model. For $n = 1, 2, \ldots$, and $j \leq n$ the evolution of clusters of mass n and diameter j due to reformation and fragmentation can be described by

$$\begin{aligned}\frac{du_{n,j}(t)}{dt} &= -(a_{n,j}+\gamma_{n,j})u_{n,j}(t) + \sum_{r=n+1}^{\infty}\sum_{s=j}^{\infty} a_{r,s}b_{n,j,r,s}u_{r,s}(t) + \gamma_{n,j+1}u_{n,j+1}(t) \\ &= -\alpha_{n,j}u_{n,j}(t) + \sum_{r=n}^{\infty}\sum_{s=j}^{\infty}\beta_{r,s}u_{r,s}(t) \qquad (28)\end{aligned}$$

where

$$\alpha_{n,j} = a_{n,j} + \gamma_{n,j} \qquad (29)$$

$$\beta_{r,s} = \begin{cases} \gamma_{n,j+1} \text{ when } r = n, s = j+1 \\ 0 \text{ when } r = n, s = j, j+2, j+3\ldots \\ a_{r,s}b_{n,j,r,s} \text{ otherwise.} \end{cases} \qquad (30)$$

Here $a_{n,j}$ is the general fragmentation rate of a cluster with mass n, diameter j and $b_{n,j,r,s}$ is the number of clusters of mass n, diameter j produced due to the break-up of a cluster of mass r, diameter s. Again $\gamma_{n,j}$ is the general reformation rate of a cluster with mass n and diameter j. For physical reasons we require

$$a_{1,1} = 0, \quad b_{n,j,r,s} = 0 \quad \text{for} \quad j > n \qquad (31)$$

and

$$\sum_{n=1}^{r-1}\sum_{j=1}^{s} n b_{n,j,r,s} = r. \qquad (32)$$

The latter relates to conservation of mass in the system. The operators A and B are now given by

$$[Af]_{n,j} := -\alpha_{n,j}f_{n,j}, \quad [Bf]_{n,j} := \sum_{r=n}^{\infty}\sum_{s=j}^{r}\beta_{r,s}f_{r,s}, \qquad (33)$$

with

$$\begin{aligned} D(A) &:= \{f \in X : \sum_{n=1}^{\infty}\sum_{j=1}^{n} n\alpha_{n,j}|f_{n,j}| < \infty\}, \\ D(B) &:= \{f \in X : \sum_{n=1}^{\infty}\sum_{j=1}^{n}\Big|\sum_{r=n}^{\infty}\sum_{s=j}^{\infty} n\beta_{r,s}f_{r,s}\Big| < \infty\}. \end{aligned} \qquad (34)$$

As before we can prove that $G = \overline{A+B}$ generates a stochastic semigroup on X and the corresponding version of Theorem 3.3 then follows.

4.2. **Coagulation with Non-Additive Diameter.** Now we examine the case where the resulting diameter after a coagulation event is not necessarily the sum of the diameters of the coagulating clusters, but can in fact take on a range of values. Consequently, after the coagulation of a cluster with mass n and diameter j with a cluster with mass r and diameter s the resulting diameter l, say, could take any value in the range $min\{j,s\} \leq l \leq j+s$. Note that we would still have the restrictions $j \leq n$ and $s \leq r$.

Previously the coagulation part of the evolution equation took the form

$$\frac{du_{n,j}(t)}{dt} = \frac{1}{2}\sum_{r=1}^{n-1}\sum_{s=1}^{j-1} k_{n-r,r,j-s,s}u_{n-r,j-s}(t)u_{r,s}(t) - \sum_{r=1}^{\infty}\sum_{s=1}^{\infty} k_{n,r,j,s}u_{n,j}(t)u_{r,s}(t). \tag{35}$$

If we are now assuming that the diameter is no longer additive the first term in (35) will change. We will now have a gain in clusters $u_{n,j}$ due to the coagulation of clusters $u_{r,l}$ and $u_{n-r,m}$ where $l < r$ and $m < n-r$. Consider the probability function, $0 \leq p'_{n,r,j,l,m} \leq 1$, which gives the probability that a cluster of diameter j will be produced by the coagulation of a cluster with mass n and diameter l with a cluster with mass r and diameter m. Note that $p'_{n,r,j,l,m} = 0$ if $j < min\{l,m\}$ or $j > l+m$. Also

$$\sum_{j=1}^{\infty} p'_{n,r,j,l,m} = 1 \quad \text{for each } n,r,l,m \tag{36}$$

and $p'_{n,r,j,l,m} = p'_{r,n,j,m,l}$ for all j. The term

$$\frac{1}{2}\sum_{r=1}^{n-1}\sum_{l=1}^{\infty}\sum_{m=1}^{\infty} k_{n-r,r,l,m}p'_{n-r,r,j,l,m}u_{n-r,l}(t)u_{r,m}(t) \tag{37}$$

will replace the first term in (35). Note that the second term will not change since the loss of clusters $u_{n,j}$ due to the coagulation of a cluster $u_{n,j}$ with another cluster will always result in a cluster with mass greater than n since mass is additive. The new evolution equation for coagulation is thus

$$\begin{aligned}\frac{du_{n,j}(t)}{dt} &= \frac{1}{2}\sum_{r=1}^{n-1}\sum_{l=1}^{\infty}\sum_{m=1}^{\infty} k_{n-r,r,l,m}p'_{n-r,r,j,l,m}u_{n-r,l}(t)u_{r,m}(t) \\ &\quad - \sum_{r=1}^{\infty}\sum_{s=1}^{\infty} k_{n,r,j,s}u_{n,j}(t)u_{r,s}(t),\end{aligned} \tag{38}$$

where we still take $d_{min}(n) = 1$ for all n. Under the assumptions that $k_{n,r,j,s}$ is symmetric in the sense that $k_{n,r,j,s} = k_{r,n,s,j}$ and is uniformly bounded by a constant k, it can be shown that there exists a global, strong, non-negative, mass-conserving solution to the ACP

$$\frac{d}{dt}u(t) = Gu(t) + Ku(t) \tag{39}$$

$$\lim_{t\to 0+} u(t) = f \in D(G)^+ \tag{40}$$

where, as before, $G = \overline{A+B}$ is the generator of the reformation (or reformation-fragmentation) semigroup.

4.3. **Discrete Mass and Continuous Diameter.** In some models, it might be more appropriate to have a cluster described by a discrete mass variable but a continuous diameter variable, in which case we would let $u_n(y)$ represent the concentration of clusters with mass $n = 1, 2, \ldots$ and diameter $y \in \mathbb{R}^+$. We shall consider the situation where the mass and diameter of a monomer have been scaled so that a particle of mass one has diameter one. Thus the largest diameter we can have in a cluster of n particles will be when the particles are joined in a single straight line and thus $u_n(y) = 0$ for $y > n$. We shall consider the coagulation equation for discrete mass and continuous diameter, which is given by

$$\begin{aligned}\frac{\partial u_n(y,t)}{\partial t} &= \frac{1}{2}\sum_{j=1}^{n-1}\int_{z=0}^{y} k_{n-j,j}(y-z,z)u_{n-j}(y-z,t)u_j(z,t)dz \\ &\quad -\sum_{j=1}^{\infty}\int_{z=0}^{\infty} k_{n,j}(y,z)u_n(y,t)u_j(z,t)dz \end{aligned} \tag{41}$$

where $k_{n,j}(y,z)$ is the coagulation rate for a cluster with mass n and diameter $y \le n$ with a cluster with mass j and diameter $z \le j$. The right-hand side of equation (41) is the analogue of (23) in the discrete case. Note that the first term is zero when $n = 1$ due to the empty sum and we have that

$$k_{n,j}(y,z) = k_{j,n}(z,y) \le k \quad \text{for all } n, j = 1, 2, \ldots \text{ and } y \le n, z \le r.$$

Note that the total mass and total diameter of the system are given respectively by

$$\sum_{n=1}^{\infty}\int_0^{\infty} nu_n(y)dy = \sum_{n=1}^{\infty}\int_0^{n} nu_n(y)dy \tag{42}$$

and

$$\sum_{n=1}^{\infty}\int_0^{\infty} yu_n(y)dy = \sum_{n=1}^{\infty}\int_0^{n} yu_n(y)dy, \tag{43}$$

and the natural space to work in is the Banach space X of all infinite sequences of real functions $\{f_n(y)\}_{n=1}^{\infty}$, $y \in \mathbb{R}^+$ such that $f_n(y) = 0$ for $y > n$ with norm

$$\|f\| := \sum_{n=1}^{\infty}\int_0^{\infty} n|f_n(y)|dy = \sum_{n=1}^{\infty}\int_0^{n} n|f_n(y)|dy < \infty.$$

If we wish to prove a theorem analogous to Theorem 3.2, then we are required to show, for example, that

$$\left\|\frac{1}{2}\sum_{j=1}^{n-1}\int_{z=0}^{y} k_{n-j,j}(y-z,z)f_{n-j}(y-z)f_j(z)dz\right\| < \infty. \tag{44}$$

This, and other similar required results, can be established in a routine manner by applying Fubini's theorem to justify interchanges in the order of summations and integrals. In the particular case of (44), we obtain

$$\left\|\frac{1}{2}\sum_{j=1}^{n-1}\int_{z=0}^{y} k_{n-j,j}(y-z,z)f_{n-j}(y-z)f_j(z)dz\right\| \le k\|f\|^2.$$

It is possible once again to show upon pairing coagulation terms with the reformation terms described previously, but within the discrete/continuous setting, that there exists a unique non-negative solution to the appropriate ACP.

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