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THE DISCRETE AGGLOMERATION MODEL: THE FIXED PROBLEM WITH APPLICATION TO THE QUADRATIC KERNEL

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Abstract

Agglomeration of particles in a fluid environment is an integral part of many industrial processes and has been the subject of scientific investigation. One model of the fundamental mathematical problem of determining the number of particles of each particle-size as a function of time for a system of particles that may agglutinate during two particle collisions uses the coagulation or Smoluchowski's equation. With initial conditions, it is called the discrete agglomeration model. Several problems have been associated with this model allowing progress to proceed separately. To facilitate this progress, in this paper, we develop and solve the fixed agglomeration problem and establish the fundamental agglomeration problem for all cases of the autonomous quadratic kernel.

1. Introduction

Agglomeration of particles in a fluid environment (e.g., a chemical reactor or the atmosphere) is an integral part of many industrial processes (e.g., Goldberger [3]) and has been the subject of scientific investigation

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(e.g., Siegell [20]). A fundamental mathematical problem is the determination of the number of particles of each *particle-type* as a function of time for a system of particles that may agglutinate during two particle collisions. Little analytical work has been done for systems where particle-type requires several variables. Efforts have focused on particle size (or mass). This allows use of the *coagulation equation* which has been well studied in aerosol research and other areas (e.g., Drake [2], Escobedo et al. [1], Leyvraz [4] and Wattis [24]). Original work on this equation was done by Smoluchowski [21] and it is also referred to as *Smoluchowski's equation*. The *agglomeration equation* is perhaps more descriptive since the term coagulation implies a process carried out until solidification whereas we focus on the agglomeration process; that is, on the determination of a time-varying *particle-size distribution* even if coagulation is never reached.

In his original work, Smoluchowski considered the agglomeration equation in a discrete form. Later it was considered in a continuous form by Müller [16]. In either case, an *initial particle-size distribution* to specify the initial number of particles for each particle size is needed to complete the *initial value problem* (IVP). We refer to these as the *discrete agglomeration model* and the *continuum agglomeration model*, respectively. Solution of either model yields an updated particle-size distribution giving *number densities* as time progresses. For various conditions, studies of these and more general models include Morganstern [11], Melzak [10], McLeod [9], Marcus [7], White [25], Spouge [22], Shirvani and Stock [18], Treat [23], Yu [26], Shirvani and Van Roessel [19], McLaughlin et al. [8] and Moseley [12-15].

Let **R** be the real numbers, $Int_O = \{I \subseteq \mathbf{R}: I$ is a finite, infinite or semi-infinite open interval$\}$ and for $I \in Int_O$, $\mathscr{A}(I, \mathbf{R}) = \{f : I \to \mathbf{R}: f$ is analytic on $I\} \subseteq C^1(I, \mathbf{R}) = \{f : I \to \mathbf{R}: f$ is continuously differential on $I\} \subseteq C(I, \mathbf{R}) = \{f : I \to \mathbf{R}: f$ is continuous on $I\} \subseteq \mathscr{F}(I, \mathbf{R}) = \{f : I \to \mathbf{R}: f$ is a function on $I\}$. If A is a subspace of a vector space B, then we write $A \subseteq_{vs} B$. These function spaces are vector spaces and $\mathscr{A}(I, \mathbf{R}) \subseteq_{vs} C^1(I, \mathbf{R}) \subseteq_{vs} C(I, \mathbf{R}) \subseteq_{vs} \mathscr{F}(I, \mathbf{R})$.

To develop the discrete model, assume that all particles are a multiple of a particle of smallest size (volume), say Δv. Thus, a particle made up of i smallest-sized particles has size $i\Delta v$. In polymer chemistry, the particle is called an *i-mer*. The initial time is $t_0 \in I_0 \in Int_o$, where I_0 is the largest time interval of interest. We use the *extended interval notation* $I_0 = (t_{0-}, t_0, t_{0+})$ and let $Int_o(I_0) = \{I \in Int_o : I \subseteq I_0\}$, and $Int_o(t_0, I_0) = \{I \in Int_o : t_0 \in I \subseteq I_0\}$. Unless otherwise specified, we assume $I \in Int_o(I_0)$. Now, for each $i \in \mathbf{N} = \{1, 2, 3, ...\}$, let $n_i(t)$ be a real-valued function (either in $C^1(1, \mathbf{R})$ or $\mathscr{A}(I, \mathbf{R})$) that approximates the number of i-mers in the reactor at time t. Since there are an infinite number of sizes, initially, we take the *state* (or *phase*) *space* to be $\mathbf{R}^\infty = \{\{a_i\}_{i=1}^\infty : a_i \in \mathbf{R}\}$. Assume the initial number density $\vec{n}_0 = \{n_i^0\}_{i=1}^\infty \in \mathbf{R}^\infty$ is known. As time passes, particles collide, agglutinations occur and larger particles result. The net rate of increase in $n_i(t)$ with time, dn_i/dt, is the rate of formation minus the rate of depletion (conservation of mass). For $I \in Int_o(t_0, I_0)$, we consider as a possible Σ space (i.e., the designated space where we look for solutions) either $\vec{\mathscr{A}}_{cw}(I, \mathbf{R}^\infty)$ for the *analytic context* or $\vec{C}^1_{cw}(I, \mathbf{R}^\infty)$ for the *continuous context* where

$$\begin{aligned}
\vec{\mathscr{A}}_{cw}(I, \mathbf{R}^\infty) &= \{\vec{n} = \{n_i(t)\}_{i=1}^\infty : n_i(t) \in \mathscr{A}(I, \mathbf{R})\} \subseteq_{vs} \vec{C}^1_{cw}(I, \mathbf{R}^\infty) \\
&= \{\vec{n} = \{n_i(t)\}_{i=1}^\infty : n_i(t) \in C^1(I, \mathbf{R})\} \subseteq_{vs} \vec{C}_{cw}(I, \mathbf{R}^\infty) \\
&= \{\vec{n} = \{n_i(t)\}_{i=1}^\infty : n_i(t) \in C(I, \mathbf{R})\} \subseteq_{vs} \vec{\mathscr{F}}(I, \mathbf{R}^\infty) \\
&= \{\vec{n} = \{n_i(t)\}_{i=1}^\infty : n_i(t) \in \mathscr{F}(I, \mathbf{R})\}.
\end{aligned}$$

Functions in $C(I, \mathbf{R})$ are continuous, but functions in $\vec{C}_{cw}(I, \mathbf{R}^\infty)$ are not as we have not established a *topology* on $\mathbf{R}^\infty$. They are *componentwise continuous*. For $\vec{n} = \{n_i(t)\}_{i=1}^\infty \in \vec{C}^1_{cw}(I, \mathbf{R}^\infty)$, we may define $d\vec{n}/dt =$

$\{dn_i/dt\}_{i=1}^{\infty}$. The derivatives dn_i/dt exist and are in $C(I, \mathbf{R})$. However, we cannot assert that $d\vec{n}/dt = \lim_{h \to 0}[(\vec{n}(t+h) - \vec{n}(t))/t]$ as we have no topology on $\mathbf{R}^{\infty}$.

Let $\mathbf{R}^{\infty \times \infty} = \{\{a_{i,j}\}_{i,j=1}^{\infty} : a_{i,j} \in \mathbf{R}\}$ be the set of "infinite matrices". The kernel (which measures adhesion or "stickiness"), $\mathbf{K}(\mathbf{t}) = \{K_{i,j}(t)\}_{i,j=1}^{\infty}$, is a doubly infinite array of real-valued functions of time either in $\mathscr{A}_{cw}(I_0, \mathbf{R}^{\infty \times \infty}) = \{\mathbf{K}(\mathbf{t}) = \{\mathbf{K}_{i,j}(\mathbf{t})\}_{i,j=1}^{\infty}$: for all $i, j \in \mathbf{N}$, $K_{i,j}(t) \in \mathscr{A}(I_0, \mathbf{R})\}$ (*analytic context*) or in $\mathbf{C}_{cw}(I_0, \mathbf{R}^{\infty \times \infty}) = \{\mathbf{K}(\mathbf{t}) = \{\mathbf{K}_{i,j}(\mathbf{t})\}_{i,j=1}^{\infty}$: for all $i, j \in \mathbf{N}$, $K_{i,j}(t) \in \mathbf{C}(I_0, \mathbf{R})\}$ (*continuous context*). As with $\mathbf{R}^{\infty}$, we establish no topology on $\mathbf{R}^{\infty \times \infty}$.

The resultant *discrete agglomeration model* or *discrete agglomeration problem* (DAP) is an IVP consisting of an infinite system of ordinary differential equations (ODE's) each with an initial condition (IC) that may be written in scalar (componentwise) form as:

$$\text{System of ODE's: } \frac{dn_i}{dt} = \frac{1}{2}\sum_{j=1}^{i-1} K_{i-j,j}(t) n_j n_{i-j} - n_i \sum_{j=1}^{\infty} K_{i,j}(t) n_j,$$

$$t \in I_0 = (t_{0-}, t_0, t_{0+}) \qquad (1.1)$$

IVP $i \in \mathbf{N} = \{1, 2, 3, ...\}$

$$\text{IC's } n_i = (t_0) = n_i^0, \quad t_0 \in I_0 \in (t_{0-}, t_0, t_{0+}), \qquad (1.2)$$

where for $i = 1$, the empty sum on the right hand side of (1.1) is assumed to be zero. The first sum in the *scalar* (componentwise) *discrete agglomeration equation* (1.1) is the (average) rate of formation of *i*-mers by agglutinations of $(i - j)$-mers with *j*-mers. The $1/2$ avoids double counting. The second sum is the (average) rate of depletion of *i*-mers by the agglutinations of *i*-mers with all particle sizes. We model a *stochastic process* as *deterministic*.

Much of the work cited above involves mathematical modeling (physics) of $\mathbf{K(t)} = \{K_{i,j}(t)\}_{i,j=1}^{\infty}$. The physical system is often *stationary* so that each $K_{i,j}$ is time independent and the model is said to be *autonomous*. In a physical context, we require $K_{i,j}(t) > 0$, $n_1^0 > 0$, and $n_i^0 \geq 0$ for $i > 1$. However, we will address DAP as a mathematical problem where we allow the initial number of particles n_i^0, the components of the kernel, $K_{i,j}(t)$, and the components of the solution, $n_i(t)$, to be negative. The physical context will be a special case.

Smoluchowski found in the physical context where $K_{i,j}(t) = A_0 > 0$ is a constant, that

$$n_i^{A_0}(t) = \left[n_i^0 + \sum_{n=1}^{i-1} \frac{k_i^{(n+1)}}{2^n} \left[\frac{A_0(t-t_0)}{1 + \frac{1}{2} M_{0,\vec{n}_0} A_0(t-t_0)} \right]^n \right] \times \frac{1}{\left(1 + \frac{1}{2} M_{0,\vec{n}_0} A_0(t-t_0)\right)^2} > 0, \quad i \in \mathbf{N} \tag{1.3}$$

with

$$k_i^{(n+1)} = \sum_{i_1+i_2+\cdots+i_{n+1}=i} n_{i_1}^0 n_{i_2}^0 \cdots n_{i_{n+1}}^0 \geq 0, \text{ and } M_{0,\vec{n}_0} = \sum_{i=1}^{\infty} n_i^0 > 0 \tag{1.4}$$

uniquely satisfies DAP on its interval of validity $I_{IV}(I_0, t_0, \vec{n}_0, A_0) \in Int_o(t_0, I_0)$. If we assume $I_0 \supseteq [t_0, \infty)$, then $[t_0, \infty) \subseteq I_{IV}(I_0, t_0, \vec{n}_0, A_0) \subseteq I_0$ as there is a lone singularity when $t = t_0 - \dfrac{2}{M_{0,\vec{n}_0} A_0} < 0$.

The infinite sum in (1.1) and the requirement on $M_{0,\vec{n}_0}$ in (1.4) (the zeroth moment of $\vec{n}$ is $M_0(t) = \sum_{j=1}^{\infty} n_j(t)$ and we require $M_{0,\vec{n}_0} = M_0(t_0)$

$= \sum_{j=1}^{\infty} n_j(t_0) = \sum_{j=1}^{\infty} n_j^0 < \infty$) motivate consideration of the Banach spaces $\ell^p =$ $\left\{ \vec{n} = \{n_i\}_{i=1}^{\infty} \in \mathbf{R}^{\infty} : \sum_{i=1}^{\infty} |n_i|^p < \infty \right\} \subseteq_{vs} \mathbf{R}^{\infty}$, where $p \geq 1$ (Martin [6, p. 3]) with norm $\| \vec{n} \|_p = \left(\sum_{i=1}^{\infty} | n_i |^p \right)^{1/p}$ (and hence a metric and a topology on $\ell^p \subseteq_{vs} \mathbf{R}^{\infty}$). Equality of two vectors in ℓ^p requires the metric (the norm of their difference) to be zero. This is equivalent to both vectors being in ℓ^p and being componentwise equal. If $(t, n) \in I \times \ell^p$, then $\| (t, n) \|_{1, p} (| t | + \| n \|_p)^{1/p}$ defines a norm on $I \times \ell^p$ (Naylor and Sell [17, p. 58]). To insure that $M_{0, \vec{n}_0}$ exists (even for negative initial conditions), we will always require $\vec{n}_0 =$ $\{n_i^0\}_{i=1}^{\infty} \in \ell^1 \subseteq_{vs} \mathbf{R}^{\infty}$ so that $\| \vec{n}(t_0) \|_1 = \sum_{i=1}^{\infty} | n_i^0 | = M_{0\vec{n}_0} < \infty$.

Moseley [12] considered the time-varying kernel $K_{i,j}(t) = A(t)$ which depends on time, but not on particle size. For this problem, in the continuous context where

$$\mathbf{K}(t) \in \mathbf{M}_{CT}(I_0, \mathbf{R}^{\infty \times \infty}) = \{\mathbf{K}(t) \in \{K_{i,j}(t)\}_{i,j=1}^{\infty}$$
$$\in \mathbf{C}_{cw}(I_0, \mathbf{R}^{\infty \times \infty}) : K_{i,j}(t) = A(t) \in C(I_0, \mathbf{R})\},$$

the problem parameters are $(I_0, t_0, \vec{n}_0, A(t)) \in Int_o \times I_0 \times \ell^1 \times C(I_0, \mathbf{R})$. In the analytic context where

$$\mathbf{K}(t) \in \mathbf{M}_{AT}(I_0, \mathbf{R}^{\infty \times \infty}) = \{\mathbf{K}(t) \in \{K_{i,j}(t)\}_{i,j=1}^{\infty}$$
$$\in \mathscr{A}_{cw}(I_0, \mathbf{R}^{\infty \times \infty}) : K_{i,j}(t) = A(t) \in \mathscr{A}(I_0, \mathbf{R})\},$$

the problem parameters are $(I_0, t_0, \vec{n}_0, A(t)) \in Int_o \times I_0 \times \ell^1 \times \mathscr{A}(I_0, \mathbf{R})$. For any kernel, solution requires that both sides of (each equation given by)

(1.1) are continuous in the continuous context and analytic in the analytic context.

The *ith depletion coefficient* associated with $t \in I_0$ and the distribution $\vec{n} = \{n_j\}_{j=1}^{\infty} \in \mathbf{R}^{\infty}$ is defined formally by the infinite series

$$f_i^d(t, \vec{n}; \mathbf{K}) = \sum_{j=1}^{\infty} K_{i,j}(t) n_j, \quad i \in \mathbf{N} = \{1, 2, 3, ...\}. \tag{1.5}$$

The only direct dependence of $f_i^d(t, \vec{n}; \mathbf{K})$ on t is through $\mathbf{K}(t)$. If (1.5) converges for all $(t, \vec{n}) \in I_0 \times \mathbf{R}^{\infty}$, then $f_i^d(t, \vec{n}; \mathbf{K})$ maps $I_0 \times \mathbf{R}^{\infty}$ to $\mathbf{R}$. We may view $f_i^d(t, \vec{n}; \mathbf{K})$ as a function of an infinite number of real variables or as a function of time and a size distribution. Regardless, if $\vec{n}(t) \in \mathscr{F}(I, \mathbf{R}^{\infty})$, and we have convergence, the composition $f_i^d(t, \vec{n}(t); \mathbf{K})$ maps I to $\mathbf{R}$. Implicit in (1.1) is that for solution in the continuous context, we must have for all $i \in \mathbf{N}$, that $f_i^d(t, \vec{n}(t); \mathbf{K}) \in C(I, \mathbf{R})$. That is, DAP requires us to first find $\vec{n}(t) \in \vec{C}_{cw}(I, \mathbf{R}^{\infty})$ such that for all $i \in \mathbf{N}$ and $t \in I$, $f_i^d(t, \vec{n}(t); \mathbf{K})$ exists (i.e., converges) and defines a function in $C(I, \mathbf{R})$. If, in addition, $\vec{n}(t) \in \vec{C}_{cw}^1(I, \mathbf{R}^{\infty})$ (the Σ space where we look for solutions) and satisfies (1.1) on I and (1.2), then it solves DAP on I. This formulation of DAP does not require mathematics beyond calculus and is often used by engineers and scientists.

For DAP with a time varying kernel, $K_{i,j}(t) = A(t)$, in the analytic context, Moseley [12] established that the more general formula

$$n_i^A(t) = \left[n_i^0 + \sum_{n=1}^{i-1} \frac{k_i^{(n+1)}}{2^n} \left[\frac{\mathscr{A}(t)}{1 + (1/2) M_{\vec{n}_0} \mathscr{A}(t)} \right]^n \right] \frac{1}{(1 + (1/2) M_{\vec{n}_0} \mathscr{A}(t))^2}, \tag{1.6}$$

where $\mathscr{A}(t) = \int_{\tau=t_0}^{\tau=t} A(\tau) d\tau$, satisfies DAP uniquely on its interval of validity

$I_{IV}(I_0, t_0, \vec{n}_0, A(t)) \in Int_o(I_0)$. For the physical context where $n_i^0 \geq 0$, $A(t) > 0$, again we have $[t_0, \infty) \subseteq I_{IV}(I_0, t_0, \vec{n}_0, A(t)) \subseteq I_0$ and require $0 \leq M_{0, \vec{n}_0} = \sum_{i=1}^{\infty} n_i^0 = \sum_{i=1}^{\infty} | n_i^0 | = \| \vec{n}(t_0) \|_1 < \infty$. The formula (1.6) satisfies (1.1) on I and (1.2) in the continuous context as well where we allow $A(t) \in C(I_0, \mathbf{R})$. However, since (1.6) was not derived using equivalent equation operations, uniqueness has not been proved rigorously for $\mathbf{K} \in \mathbf{M}_{CT}(I_0, \mathbf{R}^{\infty\times\infty})$. A step in this direction is given by Moseley [14].

Moseley [12] divided DAP into several problems which may be considered separately. Under certain conditions, a change of (both the independent and dependent) variables using (1.5) transforms DAP with a time varying kernel (Moseley [12]) into another IVP which Moseley called the *fundamental agglomeration problem* (FAP). The solution process for FAP is fully documented in Moseley [13]. For FAP, Moseley established existence and uniqueness for both the analytic and continuous contexts by using a sequential solution. He then used a generating function to obtain an explicit solution. Recursive methods using moments have been developed for DAP with an arbitrary initial condition for special cases of as well as the general quadratic or bilinear kernel (Lu [5]):

$$K_{i,j} = A_0 + B_0(i + j) + C_0 ij, \qquad A_0, B_0, C_0 \in \mathbf{R}$$

Quadratic or bilinear kernel. (1.7)

Quadratic kernels arise in applications. They represent a certain kind of polymer formation (Ziff [27]) and approximate a combination of Brownian and shear-stress coagulation (Drake [2]).

Special cases are:

$$K_{i,j} = A_0, \quad B_0 = C_0 = 0 \qquad \text{Constant kernel} \quad (1.8)$$

$$K_{i,j} = A_0 + B_0(i + j), \quad C_0 = 0 \qquad \text{Linear kernel} \quad (1.9)$$

$$K_{i,j} = B_0(i + j), \quad A_0 = C_0 = 0 \qquad \text{Sum kernel} \quad (1.10)$$

$$K_{i,j} = C_0 ij, \quad A_0 = B_0 = 0 \ (E_0 = 0, C_0 = F_0^2) \ \text{Product kernel} \quad (1.11)$$

$$K_{i,j} = ((E_0 + F_0 i)(E_0 + F_0 j)), \quad A_0 = E_0^2, B_0 = E_0 F_0, C_0 = F_0^2$$

Polymer kernel. (1.12)

Shirvani and Stock [18] obtained rather complicated formulas for the solution of Smoluchowski's equation with an autonomous quadratic (bilinear) kernel. Shirvani and Van Roessel [19] explain that the solutions can exhibit one of the following types of behavior: conservation of mass for all time, conservation of mass for a finite time only, or instantaneous gelation.

To facilitate further progress with the goal of solving DAP with a time-varying polynomial kernel, Moseley [15] developed and solved the moment problem (MP) for DAP with an autonomous quadratic kernel. The depletion coefficient containing moments is to be used to obtain FAP for various kernels. In this paper, we develop and solve the fixed agglomeration problem (FiAP) recursively and then establish FAP for the cases of the autonomous quadratic kernel given in Moseley [15]. Again, we hope to provide clear formulas for these cases using a generating formula and move toward time-varying polynomial kernels.

Hence we extend the quadratic kernel to time varying kernels where $A(t)$, $B(t)$, and $C(t) \in (I_0, \mathbf{R})$ or $C(I_0, \mathbf{R})$:

$$K_{i,j} = A(t) + B(t)(i + j) + C(i)ij, \quad \text{Time varying quadratic kernel} \quad (1.13)$$

$$K_{i,j} = A(t), \quad B(t) = C(t) = 0 \quad \text{Time varying kernel} \quad (1.14)$$

$$K_{i,j} = A(t) + B(t)(i + j), \quad C(t) = 0 \quad \text{Time varying linear kernel} \quad (1.15)$$

$$K_{i,j} = B(t)(i + j), \quad A(t) = C(t) = 0 \quad \text{Time varying sum kernel} \quad (1.16)$$

$$K_{i,j} = Cij(t), \quad A(t) = B(t) = 0 \ (E(t) = 0, C(t) = F(t)^2)$$

Time varying product kernel (1.17)

$$K_{i,\,j} = ((E(t) + F(t)i)(E(t) + F(t)\,j)), \quad A(t) = E(t)^2,\ B(t) = E(t)F(t),$$

$$C(t) = F(t)^2 \quad \text{Time varying polymer kernel.} \quad (1.18)$$

Note that a time-varying quadratic kernel is symmetric as $K_{j,\,i}(t) = A(t) + B(t)(\,j + i) + C(t)\,ji = K_{i,\,j}(t)$.

2. The Fixed Agglomeration Problem (FiAP)

We now rewrite (1.1) as the system of ODE's:

$$\frac{dn_i}{dt} + n_i\,p_i(t) = g_{i-1}(t), \qquad t \in I_0 = (t_{0-},\, t_0,\, t_{0+}), \tag{2.1}$$

where

$$p_i(t) = \sum_{j=1}^{\infty} K_{i,\,j}(t)n_j = f_i^d(\vec{n}(t); \mathbf{K}), \tag{2.2}$$

$$g_{i-1}(t) = \frac{1}{2}\sum_{j=i}^{i-1} K_{i-j,\,j}(t)n_j n_{i-j}. \tag{2.3}$$

We now cease to require (2.2) and define the IVP (2.1) and (1.2) to be the fixed agglomeration problem (FiAP) with an arbitrary $\vec{p}(t) = \{p_i(t)\}_{i=1}^{\infty}$ but maintain $g_{i-1}(t)$ as (2.3). Hence we may consider FiAP with $\vec{p}(t) \in \vec{C}_{cw}(I, \mathbf{R}^{\infty})$ and $\mathbf{K(t)} \in \mathbf{C}_{cw}(I_0, \mathbf{R}^{\infty\times\infty})$ (continuous context) or $\vec{p}(t) \in \mathscr{A}_{cw}(I, \mathbf{R}^{\infty})$ and $\mathbf{K(t)} \in \mathscr{A}_{cw}(I_0, \mathbf{R}^{\infty\times\infty})$ (analytic context). Note that FiAP has no infinite series. Following Moseley [13], when we insert an appropriate $\vec{p}(t) = \{p_i(t)\}_{i=1}^{\infty}$ for a particular kernel, we refer to (2.1) and (1.2) as the fundamental agglomeration problem (FAP) for this particular kernel. In this paper, we solve FiAP recursively in both contexts and establish FAP for the kernels given in Moseley [15].

To establish existence and uniqueness of the solution to FiAP, we establish a recursive algorithm. For $i = 1$ and 2, we use any elementary differential equations text to obtain

$$n_1(t) = n_1^0 \exp\left\{-\int_{s=n_1^0}^{s=x} p_1(s)ds\right\},$$

$$n_2(t) = n_2^0 \exp\left\{-\int_{s=t_0}^{s=t} p_2(s)ds\right\}$$

$$+\frac{1}{2}\int_{s=t_0}^{s=t} K_{1,1}(s)n_1^2(s)\exp\left\{\int_{r=t}^{r=s} p_2(r)dr\right\}ds. \quad (2.4)$$

In general, (2.1) can be solved to obtain

$$n_i(t) = n_i^0 \exp\left\{-\int_{s=t_0}^{s=t} p_i(s)ds\right\}$$

$$+\frac{1}{2}\sum_{j=i}^{i-1}\int_{s=t_0}^{s=t} K_{i-j,\,j}(s)n_j(s)n_{i-j}(s)\exp\left\{\int_{r=t}^{r=s} p_i(r)dr\right\}ds. \quad (2.5)$$

This establishes existence and uniqueness for FiAP. Later, we plan to establish existence and uniqueness for DAP by establishing that, with appropriate choice(s) of $p_i(t)$ for a particular kernel yielding a particular FAP, DAP is equivalent to this FAP.

Alternately, we may use the substitution $\widetilde{x}_i(t) = \mu_{p_i} n_i(t)$ and rewrite (2.1) as

$$\frac{d(\widetilde{x}_i(t))}{dt} = \mu_{p_i}(t)g_{i-1}(t) = g_{i-1}(t)\exp\left\{\int_{s=t_0}^{s=t} p_i(s)ds\right\} \quad (2.6)$$

which may be solved to obtain

$$\widetilde{x}_i(t) = n_i^0 + \frac{1}{2}\sum_{j=1}^{i-1}\int_{s=t_0}^{s=t} K_{i-j,\,j}(s)\widetilde{x}_j(s)\widetilde{x}_{i-j}(s)$$

$$\times\exp\left\{\int_{r=t_0}^{r=s}(p_i(r) - p_j(r) - p_{i-j}(r))dr\right\}ds. \quad (2.7)$$

If $p_i(t)$ is monotonic and not dependent on i (e.g., the positive constant coefficient kernel), we may let

$$\tau = \sigma(t) = \exp\left\{\int_{r=t_0}^{r=s} (p_i(r))dr\right\} = \exp\left\{\int_{r=t_0}^{r=s} (p(r))dr\right\}. \tag{2.8}$$

We may then let $t = \sigma^{-1}(\tau)$ to obtain

$$\tilde{x}_i(t) = n_i^0 + \frac{1}{2}\sum_{j=1}^{i-1}\int_{s=t_0}^{s=t} K_{i-j,\,j}(s)\tilde{x}_j(s)\tilde{x}_{i-j}(s)$$

$$\times \exp\left\{-\int_{r=t_0}^{r=s} (p(r))dr\right\} ds$$

$$= n_i^0 + \frac{1}{2}\sum_{j=1}^{i-1}\int_{s=t_0}^{s=t} \frac{K_{i-j,\,j}(s)\tilde{x}_j(s)\tilde{x}_{i-j}(s)}{\sigma^{-1}(s)} ds. \tag{2.9}$$

We also refer to (2.6) and the initial condition's

$$\text{IC's } \tilde{x}_i(t_0) = n_i^0, \qquad t_0 \in I_0 = (t_{0-}, t_0, t_{0+}) \tag{2.10}$$

as the fixed agglomeration problem (FiAP).

3. Selection of $\vec{p}(t)$ for a Time-varying Quadratic Kernel

The plan for solution of DAP requires computation of the depletion coefficient and then selecting $\vec{p}(t) = \{p_i(t)\}_{i=1}^{\infty}$ without first obtaining the particle size distribution $\vec{n} = \{n_j\}_{j=1}^{\infty}$. Formally, for DAP with a non-autonomous quadratic kernel, $K_{i,\,j}(t) = A(t) + B(t)(i + j) + C(t)ij$, we have

$$f_i^d(\vec{n}(t); \mathbf{K}) = \sum_{j=1}^{\infty} K_{i,\,j}(t)n_j(t) = \sum_{j=1}^{\infty} (A(t) + B(t)(i + j) + C(t)ij)n_j(t)$$

$$= (A(t) + iB(t))M_0(t) + (B(t) + iC(t))M_1(t), \quad i \in \mathbf{N}, \quad t \in I_0, \tag{3.1}$$

where $M_0(t) = \sum_{j=1}^{\infty} n_j(t)$ is the zeroth moment of $\vec{n}(t)$ (total number of particles) and $M_1(t) = \sum_{j=1}^{\infty} jn_j(t)$ is the first moment of $\vec{n}(t)$ (which is proportional to total mass). Hence if we can solve for $M_0(t)$ and $M_1(t)$, we have $f_i^d(t, \vec{n}(t); \mathbf{K})$. Moseley [15] solved the moment problem (MP) for the autonomous quadratic kernel.

In the physical case, $M_0(t)$ is always decreasing and $M_0(t)$ is bounded below by one. However, we allow fractions of particles so that $M_0(t) \geq 0$ and the point t_{M_0} occurs if and when $M_0(t) = 0$. We recall from Moseley [15] that if $\mathbf{K}(t)$ is symmetric, then $M_1(t)$ is constant. Since the non-autonomous quadratic kernel is symmetric, we have

$$M_1(t) = \sum_{j=1}^{\infty} jn_j(t) = M_1(t_0) = \sum_{j=1}^{\infty} jn_j^0(t) = M_{1, \vec{n}_0} \tag{3.2}$$

so that

$$f_i^d(\vec{n}(t); \mathbf{K}) = (A(t) + iB(t))M_0(t) + (B(t) + iC(t))M_{1, \vec{n}_0}, \quad i \in \mathbf{N}, t \in I_0. \tag{3.3}$$

Following (1.4) we require not only $M_0(t_0) \in \ell^1$,

$$\left(\| M_0(t_0) \| = \sum_{j=1}^{\infty} | n_j(t_0) | = \sum_{j=1}^{\infty} | n_j^0 | < \infty \right),$$

but also $M_1(t_0) \in \ell^1$, $\left(\| M_1(t) \|_1 = \sum_{j=1}^{\infty} j| n_j(t_0) | = \sum_{j=1}^{\infty} j| n_j^0 | < \infty \right)$.

For the zero kernel, $A(t) = B(t) = C(t) = 0$, $g_i(t) = 0$, and $M_0(t) = \sum_{j=1}^{\infty} n_j^0 = M_{0, \vec{n}_0} < \infty$, and we choose $p_i(t) = 0$. Then FiAP becomes FAPZK with solution $n_i(t) = n_i^0 =$ constant for all *i*.

4. Selection of $\vec{p}(t)$ for an Autonomous Quadratic Kernel

For the autonomous quadratic kernel, we choose

$$p_i(t) = f_i^d(\vec{n}(t); \mathbf{K}) = (A_0 + B_0 i)M_0(t) + (B_0 + C_0 i)M_{1,\vec{n}_0}, \ \ i \in \mathbf{N}, t \in I_0. \tag{4.1}$$

with $M_0(t)$ from Moseley [14]. For the constant kernel, $(A_0 \neq 0, \ B_0 = C_0 = 0)$, from Moseley [15],

$$M_0(t) = \frac{2M_{0,\vec{n}_0}}{2 + M_{0,\vec{n}_0} A_0 (t - t_0)} \tag{4.2}$$

so that we choose

$$p_i(t) = A_0 \frac{2M_{0,\vec{n}_0}}{2 + M_{0,\vec{n}_0} A_0 (t - t_0)}, \quad i \in \mathbf{N}, t \in I_0. \tag{4.3}$$

Hence FiAP becomes FAPCK where we replace (2.1) with the system of ODE's:

$$\frac{dn_i}{dt} + n_i \left(A_0 \frac{2M_{0,\vec{n}_0}}{2 + M_{0,\vec{n}_0} A_0 (t - t_0)} \right) = g_{i-1}(t),$$

$$t \in I_0 = (t_{0-}, t_0, t_{0+}), \quad i \in \mathbf{N}. \tag{4.4}$$

For the sum kernel $(A_0 = C_0 = 0, \ B_0 \neq 0)$ from Moseley [15],

$$M_0(t) = M_{0,\vec{n}_0} e^{-M_{0,\vec{n}_0} B_0 (t - t_0)} \tag{4.5}$$

so that we choose

$$p_i(t) = B_0 i M_{0,\vec{n}_0} e^{-M_{1,\vec{n}_0} B_0 (t - t_0)} + B_0 M_{1,\vec{n}_0}, \quad i \in \mathbf{N}, t \in I_0. \tag{4.6}$$

Hence FiAP becomes FAPSK where we replace (2.1) with the system of ODE's:

$$\frac{dn_i}{dt} + n_i (B_0 i M_{0,\vec{n}_0} e^{-M_{1,\vec{n}_0} B_0 (t - t_0)} + B_0 M_{1,\vec{n}_0}) = g_{i-1}(t), \quad t \in I_0. \tag{4.7}$$

For the product kernel $(A_0 = B_0 = 0,\ C_0 \neq 0)$ from Moseley [15],

$$M_0(t) = M_{0,\vec{n}_0} - \frac{1}{2}C_0(M_{1,\vec{n}_0})^2(t - t_0) \tag{4.8}$$

so that we choose

$$p_i(t) = C_0 i M_{1,\vec{n}_0}, \quad i \in \mathbf{N},\ t \in I_0. \tag{4.9}$$

Hence FiAP becomes FAPPK where we replace (2.1) with the system of ODE's:

$$\frac{dn_i}{dt} + n_i(C_0 i M_{1,\vec{n}_0}) = g_{i-1}(t), \quad i \in \mathbf{N},\ t \in I_0. \tag{4.10}$$

For the sum plus product kernel $(A_0 = 0,\ B_0 \neq 0,\ C_0 \neq 0)$ from Moseley [15],

$$M_0(t) = \left(M_{0,\vec{n}_0} + \frac{C_0}{2B_0}M_{1,\vec{n}_0}\right)e^{-B_0 M_{1,\vec{n}_0}(t-t_0)} - \frac{C_0}{2B_0}M_{1,\vec{n}_0}, \quad i \in \mathbf{N},\ t \in I_0 \tag{4.11}$$

so that we choose

$$p_i(t) = B_0 i\left(\left(M_{0,\vec{n}_0} + \frac{C_0}{2B_0}M_{1,\vec{n}_0}\right)e^{-B_0 M_{1,\vec{n}_0}(t-t_0)} - \frac{C_0}{2B_0}M_{1,\vec{n}_0}\right) + (B_0 + C_0 i)M_{1,\vec{n}_0}, \quad i \in \mathbf{N},\ t \in I_0. \tag{4.12}$$

Hence FiAP becomes FAPSPPK where we replace (2.1) with the system of ODE's:

$$\frac{dn}{dt} + n\left[B_0 i\left(\frac{C_0}{2B_0}M_{1,\vec{n}_0} + \left(M_{0,\vec{n}_0} + \frac{C_0}{2B_0}M_{1,\vec{n}_0}\right)e^{-B_0 M_{1,\vec{n}_0}(t-t_0)}\right) + (B_0 + C_0 i)M_{1,\vec{n}_0}\right] = g_{i-1}(t), \quad i \in \mathbf{N},\ t \in I_0. \tag{4.13}$$

For the linear kernel $(A_0 \neq 0,\ B \neq 0,\ C_0 = 0)$ from Moseley [15],

$$M_0(t) = \frac{2B_0 M_{0,\vec{n}_0} M_{1,\vec{n}_0} e^{-M_{1,\vec{n}_0}B_0(t-t_0)}}{2B_0 M_{1,\vec{n}_0} + A_0 M_{0,\vec{n}_0}(1 - e^{-M_{1,\vec{n}_0}B_0(t-t_0)})}, \quad i \in \mathbf{N},\ t \in I_0 \tag{4.14}$$

so that we choose

$$p_i(t) = (A_0 + B_0 i)\frac{2B_0 M_{1,\vec{n}_0} M_{1,\vec{n}_0} e^{-M_{1,\vec{n}_0} B_0 (t-t_0)}}{2B_0 M_{1,\vec{n}_0} + A_0 M_{0,\vec{n}_0}(1 - e^{-M_{1,\vec{n}_0} B_0 (t-t_0)})} + B_0 M_{1,\vec{n}_0},$$

$$i \in \mathbf{N},\ t \in I_0. \quad (4.15)$$

Hence FiAP becomes FAPLK where we replace (2.1) with the system of ODE's:

$$\frac{dn_i}{dt} + n_i\left((A_0 + B_0 i)\frac{2B_0 M_{0,\vec{n}_0} M_{1,\vec{n}_0} e^{-M_{1,\vec{n}_0} B_0 (t-t_0)}}{2B_0 M_{1,\vec{n}_0} + A_0 M_{0,\vec{n}_0}(1 - e^{-M_{1,\vec{n}_0} B_0 (t-t_0)})} + B_0 M_{1,\vec{n}_0} \right)$$

$$= g_{i-1}(t), \quad i \in \mathbf{N},\ t \in I_0. \quad (4.16)$$

For the autonomous quadratic kernel case 1, $(A_0 \neq 0,\ B_0^2 > A_0 C_0)$, we have from Moseley [15],

$$M_0(t) = \frac{r_1(M_{0,\vec{n}_0} - r_2) - r_2(M_{0,\vec{n}_0} - r_1)e^{-\frac{1}{2}A_0(r_2 - r_1)(t-t_0)}}{M_{0,\vec{n}_0} - r_2 - (M_{0,\vec{n}_0} - r_1)e^{-\frac{1}{2}A_0(r_2 - r_1)(t-t_0)}},\ \ i \in \mathbf{N},\ t \in I_0, \quad (4.17)$$

where

$$r_1 = -\frac{B_0 M_{1,\vec{n}_0} + | M_{1,\vec{n}_0} |\sqrt{B_0^2 + A_0 C_0}}{A_0},$$

$$r_2 = -\frac{B_0 M_{1,\vec{n}_0} - | M_{1,\vec{n}_0} |\sqrt{B_0^2 + A_0 C_0}}{A_0} \quad (4.18)$$

so that we choose

$$p_i(t) = (A_0 + B_0 i)\frac{r_1(M_{0,\vec{n}_0} - r_2) - r_2(M_{0,\vec{n}_0} - r_1)e^{-\frac{1}{2}A_0(r_2 - r_1)(t-t_0)}}{M_{0,\vec{n}_0} - r_2 - (M_{0,\vec{n}_0} - r_1)e^{-\frac{1}{2}A_0(r_2 - r_1)(t-t_0)}}$$

$$+ (B_0 + C_0 i)M_{1,\vec{n}_0}, \quad i \in \mathbf{N},\ t \in I_0. \quad (4.19)$$

Hence FiAP becomes FAPAQKC1 where we replace (2.1) with the system of ODE's:

$$\frac{dn_i}{dt} + n_i\left((A_0 + B_0 i)\frac{r_1(M_{0,\vec{n}_0} - r_2) - r_2(M_{0,\vec{n}_0} - r_1)e^{-\frac{1}{2}A_0(r_2-r_1)(t-t_0)}}{M_{0,\vec{n}_0} - r_2 - (M_{0,\vec{n}_0} - r_1)e^{-\frac{1}{2}A_0(r_2-r_1)(t-t_0)}}\right.$$

$$\left. + (B_0 + C_0 i)M_{1,\vec{n}_0}\right) = g_{i-1}(t), \quad i \in \mathbf{N},\ t \in I_0. \tag{4.20}$$

For the autonomous quadratic kernel case 2, $(A_0 \neq 0,\ B_0^2 = A_0 C_0)$, we have from Moseley [15],

$$M_0(t) = \frac{2A_0 M_{0,\vec{n}_0} - (B_0 M_{0,\vec{n}_0})(A_0 M_{0,\vec{n}_0} + B_0 M_{1,\vec{n}_0})(t - t_0)}{2A_0 + A_0(A_0 M_{0,\vec{n}_0} + B_0 M_{1,\vec{n}_0})(t - t_0)},$$

$$i \in \mathbf{N},\ t \in I_0 \tag{4.21}$$

so that we choose

$$p_i(t) = (A_0 + B_0 i)\frac{2A_0 M_{0,\vec{n}_0} - (B_0 M_{1,\vec{n}_0})(A_0 M_{0,\vec{n}_0} + B_0 M_{1,\vec{n}_0})(t - t_0)}{2A_0 + A_0(A_0 M_{0,\vec{n}_0} + B_0 M_{1,\vec{n}_0})(t - t_0)}$$

$$+ (B_0 + C_0 i)M_1(t_0), \quad i \in \mathbf{N},\ t \in I_0. \tag{4.22}$$

Hence FiAP becomes FAPAQKC2 where we replace (2.1) with the system of ODE's:

$$\frac{dn_i}{dt} + n_i\left((A_0 + B_0 i)\frac{2A_0 M_{0,\vec{n}_0} - (B_0 M_{1,\vec{n}_0})(A_0 M_{0,\vec{n}_0} + B_0 M_{1,\vec{n}_0})(t - t_0)}{2A_0 + A_0(A_0 M_{0,\vec{n}_0} + B_0 M_{1,\vec{n}_0})(t - t_0)}\right.$$

$$\left. + (B_0 + C_0 i)M_{1,\vec{n}_0}\right) = g_{i-1}(t), \quad i \in \mathbf{N},\ t \in I_0. \tag{4.23}$$

For the autonomous quadratic kernel case 3, $(A_0 \neq 0,\ B_0^2 < A_0 C_0)$, we have from Moseley [15],

$$M_0(t) = -\frac{B_0 M_{1,\vec{n}_0}}{A_0}$$

$$+ d_0 \tan\left(-\frac{A_0}{2} d_0 (t - t_0) + \operatorname{Arctan}\left(\frac{A_0 M_{0,\vec{n}_0} + B_0 M_{1,\vec{n}_0}}{A_0 d_0}\right)\right)$$

$$i \in \mathbf{N},\ t \in I_0, \qquad (4.24)$$

where

$$d_0 = \frac{\sqrt{A_0 C_0 - B_0^2}}{|A_0|} | M_{1,\vec{n}_0} | > 0 \qquad (4.25)$$

so that we choose

$$p_i(t) = (A_0 + B_0 i)\left(-\frac{B_0 M_{1,\vec{n}_0}}{A_0} + d_0 \tan\left(-\frac{A_0}{2} d_0 (t - t_0)\right.\right.$$

$$\left.\left. + \operatorname{Arctan}\left(\frac{A_0 M_{0,\vec{n}_0} + B_0 M_{1,\vec{n}_0}}{A_0 d_0}\right)\right)\right) + (B_0 + C_0 i) M_{1,\vec{n}_0},$$

$$i \in \mathbf{N},\ t \in I_0. \qquad (4.26)$$

Hence FiAP becomes FAPAQKC3 where we replace (2.1) with the system of ODE's:

$$\frac{dn_i}{dt} + n_i\left((A_0 + B_0 i)\left(-\frac{B_0 M_{1,\vec{n}_0}}{A_0} + d_0 \tan\left(-\frac{A_0}{2} d_0 (t - t_0)\right.\right.\right.$$

$$\left.\left.\left. + \operatorname{Arctan}\left(\frac{A_0 M_{0,\vec{n}_0} + B_0 M_{1,\vec{n}_0}}{A_0 d_0}\right)\right)\right) + (B_0 + C_0 i) M_{1,\vec{n}_0}\right) = g_{i-1}(t),$$

$$i \in \mathbf{N},\ t \in I_0. \qquad (4.27)$$

5. Summary and Future Work

We have formulated and solved recursively the fixed agglomeration problem (FiAP). Also, the fundamental agglomeration problems (FAP's) for all cases of the autonomous quadratic kernel are established. It remains to

1. establish that each of these FAP's is equivalent to their corresponding DAP's so that uniqueness is established for DAP,
2. use, if possible, generating functions to obtain explicit formulas for the solutions to the FAP's and hence for each of the DAP's,
3. verify directly that the formulas for the FAP's are correct for each DAP.

We hope to accomplish this for each FAP and hence each DAP for the autonomous quadratic kernel and for at least some cases of the non-autonomous quadratic and perhaps polynomial kernels in the future.

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