The Discrete Unbounded Coagulation-Fragmentation Equation with Growth, Decay and Sedimentation

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Content

Focus of Presentation

1. In this presentation, we study the discrete coagulation–fragmentation models with growth, decay and sedimentation. We demonstrate the existence and uniqueness of classical global solutions, using the theory of linear and semilinear semigroups of operators, provided the linear processes are sufficiently strong.
2. The conclusions obtained from the theories are supported by numerical simulations.

Applications

- In the applications of coagulation-fragmentation models to life sciences, the clusters consist of living organisms and can change their size not only due to the coalescence or splitting, but also due to internal demographic processes such as death or birth of organisms inside.
- Specifically, in the phytoplankton dynamics, the removal of whole clusters due to their sedimentation is an important process that is responsible for rapid clearance of the organic material from the surface of the sea.
- The removal of clusters of suspended solid particles from a mixture is also important in water treatment, biofuel production, or beer fermentation.

The Phytoplankton

- Phytoplankton serves as the oxygen-producing foundation of many marine food chains and humans (about 50% of the world's oxygen).
- Aggregates of phytoplankton are formed due to collisions of smaller aggregates and due to their stickiness resulting from the presence of organic glues such as carbohydrates and Transparent Exopolymer Particles (TEP).
- Jackson (1990) in modelling the dynamics of Phytoplankton,

$$
\begin{aligned}
\frac{d}{dt}C_1 &= \mu C_1 - \alpha C_1 \sum_{i=1}^{\infty} C_i \beta_{1,i} - \frac{C_1 w_i}{z}, \\
\frac{d}{dt}C_n &= \frac{\alpha}{2} \sum_{i=1}^{n-1} C_i C_{n-i} \beta_{i,n-i} - \alpha C_n \sum_{i=1}^{\infty} C_i \beta_{n,i} - \underbrace{\frac{C_n w_n}{z}}_{\text{sedimentation of aggregate}}, \quad n \geq 2.
\end{aligned}
$$

  He suggested a generalization of the above model.
- Hence, the model should include fragmentation, growth and death terms

The full Model

The full model, [Banasiak J.], would be:

$$
\begin{aligned}
\frac{df_i}{dt} &= \underbrace{(g_{i-1}f_{i-1} - g_i f_i)}_{\text{growth of a cell}} \\
&\quad \underbrace{+(d_{i+1}f_{i+1} - d_i f_i)}_{\text{death of a cell (decay)}} \quad \underbrace{-s_i f_i}_{\text{death of aggregate (sedimentation)}} \\
&\quad \underbrace{-a_i f_i + \sum_{j=i+1}^{\infty} a_j b_{i,j} f_j}_{\text{Fragmentation of aggregate}} \qquad (1) \\
&\quad \underbrace{+\frac{1}{2}\sum_{j=1}^{i-1} k_{i-j,j} f_{i-j} f_j - \sum_{j=1}^{\infty} k_{i,j} f_i f_j,}_{\text{coagulation of aggregate}} \quad i \geq 1, \\
f_i(0) &= f_i^0, \quad i \geq 1.
\end{aligned}
$$

Assumptions

- As clusters can fragment into two or more smaller pieces (multiple fragmentation) but not into bigger clusters, we note the following:

$$\begin{aligned} & a_1 = 0, \quad a_i \geq 0 \in \mathbb{R}, \quad i \geq 2, \\ & b_{1,j} = 0, \\ & b_{i,j} = 0, \quad j \geq i. \end{aligned} \tag{2}$$

- Naturally, for this system to conserve mass, the following assumption has to be imposed

$$\sum_{i=1}^{j-1} i b_{i,j} = j, \quad j \geq 2. \tag{3}$$

- From the physical point of view, both the fragmentation term and the coagulation term should be symmetric.

Literature

- The discrete model is not as popular in the literature as the continuous model. We decided to contribute to the discrete case.
- For the continuous case, some authors (Arlotti & Banasiak, 2004; Banasiak & Lamb, 2003 & 2009; Banasiak, 2006; Banasiak & Oukouomi, 2009; Cai et al, 1991; Edwards et al, 1990; Huang et al, 1991; Mischler & Scher, 2016; Omari, 2011; Poka, 2012;) have worked on equation (1) with either
  - the decay, sedimentation and coagulation terms are not included, or
  - the growth and sedimentation terms are not included
- Smith et al (2011), worked on the discrete equation of (1) but with a bounded coagulation term and without the growth and sedimentation term using the discrete form of the mass loss condition

$$\sum_{n=1}^{j-1} nb_{n,j} = j(1-\lambda_j) \quad \text{for} \quad j \geq 2. \tag{4}$$

Abstract Cauchy Problem

Formulating the equation as an Abstract Cauchy Problem (ACP):

$$\frac{df}{dt} = Y_p f + K_p f, \quad f(0) = (f_n)_n^\infty. \tag{5}$$

where Y_p is the linear part, and K_p is the nonlinear part

$$\begin{aligned}[Y_p f]_i &= g_{i-1} f_{i-1} - (g_i + d_i + s_i + a_i) f_i, \quad i \geq 1, \quad a_1 = 0, \\ &+ d_{i+1} f_{i+1} + \sum_{j=i+1}^{\infty} a_j b_{i,j} f_j, \quad i \geq 2.\end{aligned} \tag{6}$$

$$[K_p f]_i = \frac{1}{2} \sum_{j=1}^{i-1} k_{i-j,j} f_{i-j} f_j - \sum_{j=1}^{\infty} k_{i,j} f_i f_j, \quad i \geq 1 \tag{7}$$

Growth-sedimentation-fragmentation equation

We shall use the fact that equation (6) can be written as the growth-sedimentation-fragmentation model

$$\frac{df_n}{dt} = g_{n-1}f_{n-1} - (g_n + \mathbf{a}_n + s_n)f_n + \sum_{i=n+1}^{\infty} \mathbf{a}_i \mathbf{b}_{n,i} f_i, \quad n \geq 1,$$

$$f_n(0) = f_n^{in}, \quad n \geq 1, \tag{8}$$

where $\mathbf{a}_n = a_n + d_n$, $n \geq 2$, (with $\mathbf{a}_1 = 0$) and

$$\mathbf{b}_{n,i} = \begin{cases} \frac{a_{n+1}b_{n,n+1}+d_{n+1}}{a_{n+1}+d_{n+1}}, & i = n+1, \\ \frac{a_i b_{n,i}}{a_i+d_i}, & i \geq n+2. \end{cases} \tag{9}$$

- We note that the fragmentation part of this model no longer is conservative as

$$\sum_{n=1}^{i-1} n\mathbf{b}_{n,i} = i\left(1 - \frac{d_i}{i(a_i + d_i)}\right), \qquad i \geq 2, \tag{10}$$

so it corresponds to the model with the so-called discrete mass-loss with mass-loss fraction $\lambda_n = d_n/n(a_n + d_n)$, (see Cai, 1991), mathematically analysed in (Smith, 2011).

- The analysis of the pure fragmentation equation most often is carried out in the space $X_1 := \ell_1^1$ with the norm

$$\|f\|_{[1]} = \sum_{n=1}^{\infty} n|f_n| \tag{11}$$

which, for a nonnegative f, gives the mass of the ensemble.

- However, it is much better to consider (1) in the spaces with finite higher moments, $X_p := \ell_p^1$, with the norm

$$\|f\|_{[p]} = \sum_{n=1}^{\infty} n^p|f_n|, \qquad p \geq 1. \tag{12}$$

Operators

We consider the operators $(T_p, D(T_p))$, $(G_p^-, D(G_p))$, $(D_p^+, D(D_p))$ and $(B_p, D(B_p))$ defined by

$$[T_p f]_i = -\theta_i f_i, \qquad [G_p^- f]_i = g_{i-1} f_{i-1},$$

$$[D_p^+ f]_i = d_{i+1} f_{i+1}, \qquad [B_p f]_i = \sum_{j=i+1}^{\infty} a_j b_{i,j} f_j, \quad i \geq 1,$$

where $\theta_i := a_i + g_i + d_i + s_i$, $i \geq 1$, and $g_0 = a_1 = 0$. Further, we denote

$$\Delta_i^{(p)} := i^p - \sum_{j=1}^{i-1} j^p b_{j,i}, \quad i \geq 2, \; p \geq 0. \tag{13}$$

Then the following holds (see Banasiak et al, 2018 for the details):

Generation of Analytic Semigroup

Theorem (1)

If for some $p > 1$

$$\liminf_{i\to\infty} \frac{a_i}{\theta_i} \frac{\Delta_i^{(p)}}{i^p} > 0, \tag{14}$$

then for any $p > 1$ *the sum* $(Y_p, D(Y_p)) = (T_p + G_p + D_p + B_p, D(T_p))$ *generates a positive analytic* C_0*-semigroup* $\{S_p(t)\}_{t\geq 0}$ *in* X_p*.*

Proof: - the diagonal operator generates a substochastic analytic semigroup

- perturbation by $[G_p^- f]$
- perturbation by $[B_p f]$, and
- by Arendt-Rhandi theorem, the sum generates an analytic semigroup

Local Mild Solution

We assume that all the conditions of Theorem 1 are satisfied. In addition, we impose the following bound on the coefficients of the coagulation kernel

$$k_{i,j} \leq \kappa((1+\theta_i)^{\alpha} + (1+\theta_j)^{\alpha}), \quad i,j \geq 1,\ 0 < \alpha < 1. \tag{15}$$

Then, we proved the following theorem
where the norm of the intermediate spaces, $X_{p,\alpha}$, is given by the expression

$$\|f\|_{p,\alpha} = \sum_{i=1}^{\infty} i^p (1+\theta_i)^{\alpha} |f_i|, \quad 0 < \alpha < 1. \tag{16}$$

Lemma (1)

Assume for some $p > 1$ conditions (14) and (15) are satisfied. Then for each $f_0 \in X_{p,\alpha}^{+}$ and some $T > 0$, the initial value problem (1) has a unique non-negative mild solution $f \in C([0,T], X_{p,\alpha})$.

Local Classical Solution

Theorem (2)

Assume that conditions (14) *and* (15) *are satisfied. Then, for each* $f_0 \in X_{p,\alpha}$ *there is* $T = T(f_0) > 0$ *such that the initial value problem* (1) *has a unique non-negative classical solution* $f \in C([0, T], X_{p,\alpha}) \cap C^1((0, T), X_p) \cap C((0, T), X_{p,1})$.

Proof: - We use the variation of constant formula
-We prove the map is bounded, locally lipschitz continuous and it is a contraction
- We prove the differentiability of the mild solution

Global Solution

Lemma (2)

Assume that $f_0 \in X^+_{p,\alpha}$ *and for some* ω_1

$$\frac{g_i - d_i}{i} - s_i \leq \omega_1 \tag{17}$$

Then, under the assumptions of Theorem (2)*, the local solution satisfies*

$$\|f\|_1 \leq e^{\omega_1 t}\|f_0\|_1, \qquad t \in (0, T(f_0)). \tag{18}$$

Theorem (3)

Under the assumptions of Theorem (2) *and Lemma* (2)*, any solution of* (1) *with* $f_0 \in X^+_{p,\alpha}$*,* $p \geq 1$*, is global in time.*

Truncated Equation

In numerical simulations, we approximate the original infinite dimensional system (1) by the following finite dimensional counterpart:

$$\begin{aligned}\frac{du_i}{dt} &= g_{i-1}u_i - \theta_i u_i + d_{i+1}u_{i+1} + \sum_{j=i+1}^{N} a_j b_{i,j} u_j \\ &\quad + \frac{1}{2}\sum_{j=1}^{i-1} k_{i-j,j}u_{i-j}u_j - \sum_{j=1}^{N} k_{i,j}u_i u_j + \frac{\delta_{N,i}}{N}\sum_{j=1}^{N}\sum_{n=N+1-j}^{N} jk_{n,j}u_n u_j, \\ u_i(0) &= u_{0,i}, \quad 1 \le i \le N.\end{aligned} \tag{19}$$

The quadratic penalty term ensures that the discrete coagulation process is conservative – this property is important when dealing with pure coagulation-fragmentation models.

We show that if $u^{(N)}$ is the solution of the truncated problem (19) with the initial condition $u_0^{(N)}$, then the sequence $I_N u^{(N)}$ approaches f as the truncation index N increases.

Solvability of the Truncated Equation

Theorem (4)

Assume (14), (15) *and* (17) *hold. The truncated problem in* (19) *is locally solvable, i.e. for each* $p > 1$ *there exists some* $T > 0$ *such that for each* N

$$u^{(N)} \in C([0,T], X_{p,\alpha}) \cap C^1((0,T), X_p) \cap C((0,T), X_{p,1}), \tag{20}$$

and the respective norms of $u^{(N)}$ *are bounded independently of* N. *If, in addition, the initial datum* $u_0^{(N)}$ *is non-negative,* (20) *holds for any fixed* $T > 0$. *Finally, if for some* $q > p-1$, $q \geq 0$ *we have* $f_0 \in X^+_{q+1,\alpha}$ *and* $\lim_{N\to\infty} \|I_N u_0^{(N)} - f_0\|_{p,\alpha} = 0$, *then* $I_N u^{(N)} \to f$ *in* $C([0,T], X_{p,\alpha})$ *as* $N \to \infty$.

Proof: See Banasiak et al, 2018

Fragmentation and Coagulation Kernels

In our simulations, we make use of the following two fragmentation kernels:

$$b_{i,j} = \frac{2}{j-1}, \tag{21a}$$

$$b_{i,j} = \frac{i^\sigma (j-i)^\sigma}{\alpha_j}, \quad \alpha_j = \frac{1}{j}\sum_{i=1}^{j-1} i^{1+\sigma}(j-i)^\sigma, \quad \sigma > -1. \tag{21b}$$

And the coagulation process is driven by one of the unbounded kernels:

$$k_{i,j} = k_1(i^{1/3} + j^{1/3})^{\frac{7}{3}}, \tag{22a}$$

$$k_{i,j} = k_2(i + k_3)(j + k_3), \tag{22b}$$

where k_1, k_2 and k_3 are positive constants.

Parameters

- The transport, the sedimentation and the fragmentation rates are chosen to be

$$g_i = gi^{\alpha}, \quad d_i = di^{\beta}, \quad s_i = si^{\gamma}, \quad a_i = ai^{\delta},$$

for all $i \geq 1$, except for $d_1 = a_1 = 0$.

- In view of Theorem (1), in the calculations below it is assumed that either

$$\max\{\alpha, \beta, \gamma\} \leq \delta, \quad p > 1, \tag{23a}$$

or

$$\max\{\beta, \delta\} \leq \gamma, \quad p = 1, \tag{23b}$$

- The conditions ensure that the associated semigroups $\{S_p(t)\}_{t\geq 0}$, equipped with either of the fragmentation kernels (21a) or (21b), are analytic in X_p, $p \geq 1$.

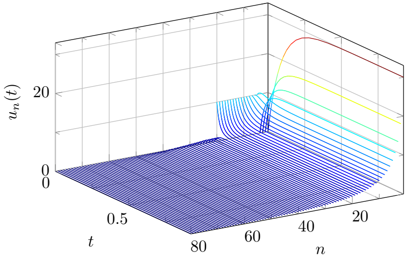
The pure coagulation-fragmentation

- To begin, we consider (1) with $g = d = s = 0$, fragmentation kernel (21a) and coagulation kernel (22a). Here, the coagulation coefficients satisfy $k_{i,j} = \mathcal{O}(i^{\frac{7}{9}} + j^{\frac{7}{9}})$ hence Threorem (3) applies, provided $\delta > \frac{7}{9}$.
- In our simulations, we let: $N = 200$, $a = 1$, $\delta = 1$ and $k_1 = 5 \cdot 10^{-3}$. Since N is fixed, we shorten the notation setting $u^N = u$. As the initial conditions, we take

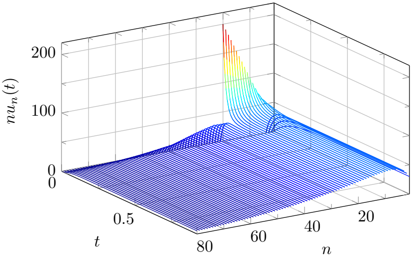
$$u_n(0) = 10, \quad 5 \leq n \leq 20 \quad \text{and} \quad u_n(0) = 0 \quad \text{otherwise}$$

  and integrate (19) in time interval $[0, 1]$ using **ode15s** built-in **Matlab** ODE solver.
- The results of the simulations are shown below.

The pure coagulation-fragmentation contd

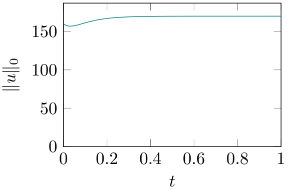


(a) Number of clusters

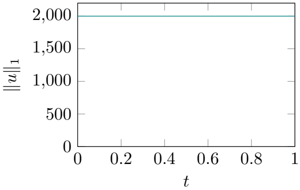


(b) Distribution of cluster masses

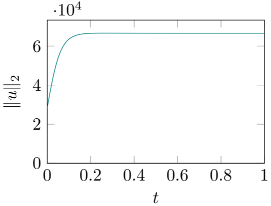
The pure coagulation-fragmentation contd 2



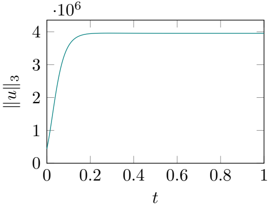
(c) Total number of particles



(d) The total mass



(e) Higher moments, $p = 2$

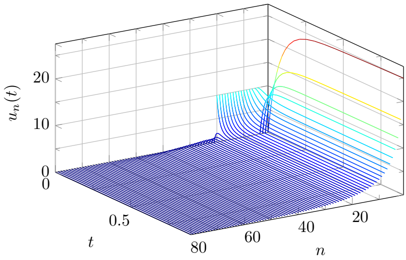


(f) Higher moments, $p = 3$

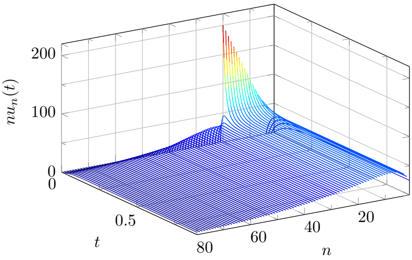
The fragmentation-coagulation equation with growth-decay-sedimentation

- We consider the complete model (1), with $g = d = s = a = 1$, $\beta = \gamma = 0$ and $\alpha = \delta = 1$.
- The fragmentation and the coagulation processes are controlled respectively by the kernels (21a) and (22a), with $k_1 = 5 \cdot 10^{-3}$.
- The truncation index N, the time interval $[0, T]$ and the initial condition u_0 are chosen to be the same as in Examples 1.
- The death and the sedimentation processes dominate and yield a slow decay in the moments as time increases.

The fragmentation-coagulation equation with growth-decay-sedimentation contd

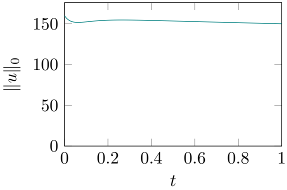


(g) Number of clusters

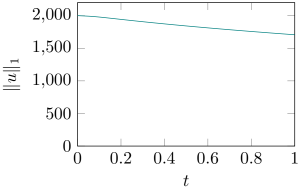


(h) Distribution of cluster masses

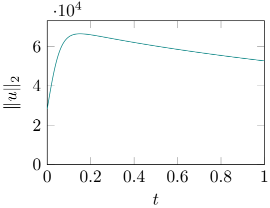
The fragmentation-coagulation equation with growth-decay-sedimentation contd 2



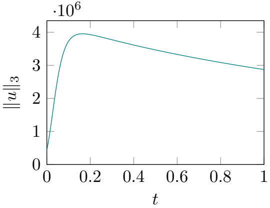
(i) Total number of particles



(j) The total mass

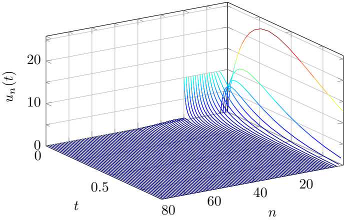


(k) Higher moments, $p = 2$

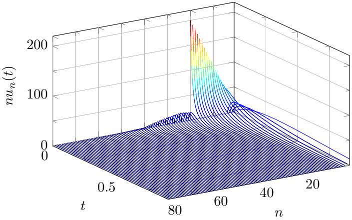


(l) Higher moments, $p = 3$

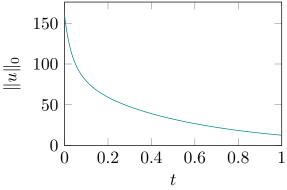
Strong Sedimentation case



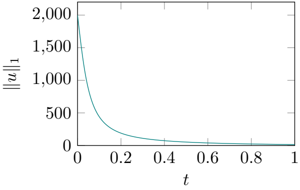
(m) Number of clusters



(n) Distribution of cluster masses



(o) Total number of particles



(p) The total mass

References

[1] Banasiak J., Joel L. O. and Shindin S. (2018) The Discrete Unbounded Coagulation-Fragmentation Equation with Growth, Decay and Sedimentation. ArXiv eprint, arXiv:1809.00046, August 2018.

[2] Banasiak J., Joel L.O. and Shindin S. (2017) Analysis and simulations of the discrete fragmentation equation with decay, Mathematical Methods in the Applied Sciences

[3] Banasiak J. (2001), On an extension of the Kato-Voigt perturbation theorem for substochastic semigroups and its application, Taiwanese Journal of Mathematics, vol 5.

[4] Banasiak J., and Lamb W. (2003), On the application of substochastic semigroup theory to fragmentation models with mass loss, Journal of mathematical analysis and applications, vol 284, pages 9–30.

[5] Banasiak J., Arlotti L. (2006), Perturbations of positive semigroups with applications, Springer Science & Business Media

[6] Cai M., Edwards B. F. and Han H. (1991), Exact and asymptotic scaling solutions for fragmentation with mass loss, Physical Review A, vol 43, pages 656 - 662.

[7] Jackson, G. A. (1990). A model of the formation of marine algal flocs by physical coagulation processes. Deep Sea Research Part A. Oceanographic Research Papers, 37(8):1197 1211.

[8] Smoluchowski M., Drei vortrage uber diffusion, brownsche bewegung und koagulation von kolloidteilchen. Zeitschrift fur Physik, 17:557-585, 1916.

[9] Pazy, A. (1983), Semigroups of linear operators and applications to partial differential equations, Applied mathematical sciences, Springer, New York, Berlin.

[10] Smith A. L., (2011), Mathematical analysis of discrete coagulation-fragmentation equations, PhD Theses, University of Strathclyde.

[11] Voigt J. (1987), On substochastic C0-semigroups and their generators, Transport Theory and Statistical Physics, vol 16, pages 453–466, Taylor & Francis.

[12] Ziff R. M. and McGrady E. D. (1985), The kinetics of cluster fragmentation and depolymerisation, Journal of Physics A: Mathematical and General, vol 18.

Thank you

Thank you!!!