SYNOPSIS OF

MATHEMATICAL STUDY OF A DISCRETE AGGREGATION MODEL

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1 INTRODUCTION

In any particulate system, the spontaneous interaction among the particles leads to a change in particulate properties such as size, mass, volume, etc. The events responsible for changing these particulate properties are known as particulate processes. Some well-known particulate processes are (i) *aggregation* or *coagulation*, and (ii) *fragmentation* or *breakage* of the particles. It is evident from the terminology that *aggregation* describes the dynamics of the formation of a larger-sized particle by combining two or more smaller-sized particles. The resulting larger particle after the aggregation process is known as an aggregate. If the total mass of the system remains constant, the aggregation process reduces the total number of particles in the system while gradually increasing the average size of the particles over time. On the other hand, *fragmentation* is the reverse phenomenon of aggregation. In the fragmentation process, particles break into smaller pieces, so this type of particulate process is also called breakage. Therefore, if the total mass of the system is conserved, fragmentation leads to an increase in the total number of particles in the system. Among these particulate processes, we will use the aggregation process as the primary mechanism to define the theme model of this thesis.

Mathematical representation of the above-mentioned particulate processes can be described by a specific kind of time evolution equations popularly known in the literature as the population balance equation (PBE). In 1916, M. von Smoluchowski first introduced the balance equation describing the conventional aggregation mechanism. Smoluchowski (1916) proposed an infinite-dimensional system of differential equations representing the discrete classical aggregation equation, also known as the *Smoluchowski aggregation equation* (SAE). In later years, the renowned mathematician Pavel V. Dubovskiĭ (1999*b*) introduced a discrete aggregation equation whose primary mechanism is different from that of SAE. The thesis deals with the dynamical model proposed by Dubovskiĭ (1999*a*,*b*), which is also referred to as the discrete *Safronov-Dubovskiĭ* aggregation equation (SDAE).

To describe the model, we consider a cluster of i number of base particles (also called monomer). This cluster is called an $i-$mer. Also, consider $a_i(t)$ to denote the concentration of the $i-$mer particles at time t in the system. Corresponding to the number density function $a_i(t)$, the discrete SDAE reads as for $i \geq 1$

$$\frac{\mathrm{d}a_i(t)}{\mathrm{d}t} = a_{i-1}(t)\sum_{j=1}^{i-1}\beta_{i-1,j}\,j a_j(t) - a_i(t)\sum_{j=1}^{i}\beta_{i,j}\,j a_j(t) - a_i(t)\sum_{j=i}^{\infty}\beta_{i,j}a_j(t), \qquad (1)$$

supported with the initial data

$$a_i(0) = a_i^0. \tag{2}$$

Here, $\beta_{i,j}$ (with $i \neq j$) represents the aggregation kernel, describing the intensity rate of the $i-$mer particle with a $j-$mer particle. In general, the aggregation kernel β is nonnegative and symmetric in nature. Moreover, for $i = j$ it is defined that the kernel $\beta_{i,i}$ equals half of the collision rates between two $i-$mers. The first sum on the right-hand side represents the inclusion of new $i-$mer particles into the system. In this regard, this term is also known as the *birth term*. On the other hand, the second and third terms describe the extraction of existing $i-$mer particles from the system at the same time t. Therefore, these terms are called *death term*.

2 MOTIVATION

The particle population balance equations are basically developed from the modeling of different types of physical phenomena and experimental process related to particle size evolution. To establish these equation, it is necessary for the study to investigate them mathematically. Among these analyzing the existence, uniqueness, nonexistence, asymptotic analysis are the most crucial investigation for a population balance equation to implement it in several field of applications.

Before the pioneer study of Dubovskiǐ (1999*a*,*b*) on the discrete SDAE, Oort and Van de Hulst (1946) introduced a continuous aggregation equation describing the aggregation process of protoplanetary bodies in astrophysics. In later years, Safronov (1972) rewrote that evolution equation in a more tractable form, enhancing its interest for applications in several fields of studies known as the *Oort-Hulst-Safronov* (OHS) aggregation equation. Afterwards, several researchers paid attention to explore various mathematical aspects like existence, self-similarity, and convergence property of the solution to the continuous OHS aggregation equation [Lachowicz *et al.* (2003); Laurençot (2005, 2006); Barik *et al.* (2022)].

To simplify the complexity of the OHS aggregation equation, Dubovskiǐ (1999*b*) first proposed the discrete aggregation equation (1) and established the connection between discrete SAE and SDAE. In the same research work, he also showed that the OHS equation is the continuous form of our considered model (1). Dubovskiǐ (1999*a*) also discussed different aspects of mass-conservation properties of the discrete SDAE (1) over different kinetic regimes. After Dubovskiǐ's works, Wattis (2012) and Davidson

(2014) have reported some recent advancements on the Safronov-Dubovskiĭ aggregation model. Wattis (2012) proposed a new discrete aggregation-fragmentation model in the light of the OHS model and analyzed the self-similar and steady-state behavior of the solution over a specific aggregation rate. Davidson (2014) investigated the basic mathematical aspects of the SDAE by analyzing the existence of the solution for some bounded aggregation rates.

The above discussion leads to the fact that the literature on the SDAE contains very few instances where the model plays a significant role in describing several physical fields of study such as astrophysics (cloud forming), cosmology (formation of planets and galaxies), astronomy (asteroid size distribution) etc. Moreover, most of the mathematical investigations on this SDAE have dealt with a bounded aggregation rate. It is very natural that the chances of the formation of large particles for a pure aggregation model are very high. This fact is well captured through the aggregation kernel having an unbounded growth rate. Furthermore, the formation or destruction rate of the protoplanetary bodies (like stars, planets, Earth, etc.) or some other industrial products depends on the size of the colliding bodies. From a mathematical point of view, it is interesting to investigate equation (1) with unbounded aggregation rates. However, the inclusion of unbounded kernels into the system may hamper the behavior of the system. In this context, a natural but important part of the study is to establish the well-posedness of the problem. Here, the well-posedness of the problem is checked by analyzing the existence and uniqueness of the solutions using sequential convergence results.

Since the particles are neither created nor destroyed in the interactions described by equation (1), it is expected that the total mass of the particles $\mathscr{Q} = \sum_{i=1}^{\infty} i a_i(t)$ should remain conserved. However, being a pure aggregation model, the discrete SDAE equation cannot produce smaller size particles to balance the particle size in the system. Therefore, there will be a high chance of a violation of mass conservation at finite time intervals. The decrease of the total mass of the system can be interpreted as the formation of infinite clusters or gel. In the literature, this finite-time breakdown of mass conservation is known as the gelation phenomenon, which plays a crucial role in several fields of applications. In this context, Van Dongen (1987) and Carr and da Costa (1992) have studied the occurrence of gelation for discrete SAE. Several other articles from different authors can be found addressing the occurrence of gelling phenomena for different particulate models [Escobedo *et al.* (2002); Lachowicz *et al.* (2003); Da Costa (2015)].

Besides the existence and uniqueness of the solution to the SDAE, investigations on mass loss behavior together with the nonexistence of the nontrivial solution to the discrete SDAE are equally necessary from the application point of view. Along with these mathematical aspects, the steady-state behavior of the solution for some specific set of kernels is another necessary theoretical aspect that enhances the applicability of the discrete SDAE. From the above-discussed literature, it is obvious that the modeling of SDAE lacks theoretical foundations in several mathematical aspects. Therefore, we choose the problem incorporating several mathematical aspects together with the aim to widen the existence theory so that it can cover most of the physically realistic kernels into consideration.

3 OBJECTIVES AND SCOPE

The objectives and scope of the present research workis segregated into four categories which we will discuss in the following points:

(i) The unbounded aggregation kernels possess much practical importance. Therefore, we aim to establish the global existence of solutions for a wide class of aggregation kernels, which covers most of the realistic kernels for experimental applications. Along with the existence result, this work proves the existing solution is mass conserving without any additional restriction on the aggregation kernel. Moreover, with some additional conditions on the initial data and aggregation kernel, we show that the obtained solution is unique.

(ii) Together with the global existence of the mass-conserving solution, mass loss phenomena is also considered for a specific set of aggregation kernels. The study successfully proves that for the considered set of aggregation rates, the mass loss event occurs at any time interval. As a consequence of this instantaneous mass loss phenomenon, the nonexistence of any non-trivial solution is proven for a set of aggregation kernels.

(iii) Note that the discrete SDAE is a pure aggregation model. In a dispersed system, only the large size particle is produced. To balance the particle size in the system, this study introduces a population balance model, which is a combination of the SDAE associated with external force where particle injection and extraction can take place. Together with the introduction of the Safronov-Dubovskiĭ aggregation equation with forcing (SDAEWF), we will also establish the well-posedness of the model. The underlying objective for studying SDAEWF is to work towards a connection with an additional differential equation, which is a common theme in the context of reaction-diffusion systems.

(iv) To provide a theoretical foundation for the SDAEWF, we establish uniqueness and continuous dependence on the initial data of the solution. Then we prove the existence of a unique equilibrium solution to the proposed SDAEWF model. Additionally, this study establishes that any solution of the SDAEWF model converges towards the equilibrium solution with an exponential convergence rate under suitable conditions on the forcing coefficients.

4 DESCRIPTION OF THE RESEARCH WORK

4.1 Existence and uniqueness of mass conserving solution

In this thesis, a comprehensive mathematical investigation is conducted on the existence and uniqueness of the strong solution to the discrete SDAE with unbounded aggregation rates. To prove the main theorem, we present the hypotheses for our problem along with some necessary definitions. Initially, we truncate the model into a finite-dimensional system. Subsequently, we prove the local existence theorem for the existence and uniqueness of a solution to the truncated system. From the local solution, we extract a sequence of solutions. With the help of some strong convergence results, we establish the existence of a convergent subsequence. Finally, we demonstrate that the limit function of the convergent subsequence is a solution to our original model. Additionally, we prove that the solutions obey the mass conservation rule for the same aggregation rates. This study is concluded by showing that solution is unique with an additional restriction on initial data and the aggregation kernel. All these results have been presented in our article Das and Saha (2021).

4.2 Instantaneous mass loss and nonexistence of nontrivial solution

This portion of the thesis focuses on the mass loss phenomena and the nonexistence of nontrivial solutions to the discrete SDAE. Initially, we discuss some preliminary definitions and properties of the solution, which are essential for the study of the gelling behavior of the solution. The proof begins by establishing the finiteness of higher-order moments of a mass-conserving solution under certain restrictions on the aggregation kernel. At the end of the proof, finiteness of moment functions, together with some additional information on the moment functions, leads us to instantaneous mass loss phenomena for that specific kind of aggregation rates. Finally, this chapter concludes with the proof of the nonexistence theorem for nontrivial solutions for a wide family of unbounded kernels. These results are published in our article Das and Saha (2022).

4.3 The discrete Safronov-Dubovskiĭ aggregation equation with forcing

To explore the steady-state behavior of the solution, we consider the SDAE with some additional forcing coefficients. This extension of the original SDAE leads us to an equilibrium solution with a specific rate of convergence. To provide a theoretical foundation for the proposed model, we start our study with some prior estimates of higher-order moments of the solutions. We truncate the model into a finite-dimensional system and prove an existence result for that truncated system. Then, we construct a sequence of functions from the solution of the truncated system. Finally, utilizing strong convergence theorems, we conclude the existence theorem by showing that the limit of one of the subsequences of the constructed sequence is a solution to the considered problem. This work is presented in the first part of our manuscript Das and Saha (2023).

4.4 Convergence to the equilibrium solution

Finally, we prove the convergence of the steady-state solution to the SDEWF, which is the primary goal of extending the SDAE with the external forcing term. To prove the existence of the equilibrium solution, we start our study by demonstrating a contraction property of the solution to the SDEWF. Relying on this contraction property, we prove the uniqueness and continuous dependence on the initial data of the global solutions to the SDAEWF model. In this way, we complete the well-posedness proof of the SDAEWF model. Finally, with some additional restrictions on the forcing coefficients, we obtain the existence of a unique equilibrium solution. We prove that any solution to the SDAEWF converges to that equilibrium solution with an exponential rate of convergence. This work has appeared in the second part of our manuscript Das and Saha (2023).

5 CONCLUSIONS

We list out the following conclusions.

1. Existence and uniqueness of global mass conserving solutions of the equation (1) for unbounded aggregation kernel is established. In particular, a convergent subsequence of a sequence of solution is obtained over a Banach space by using Arzela-Ascoli theorem. It is proved that the limit function obtained from the convergent subsequence is the actual solution of the discrete SDAE (1). The uniqueness of the solution is also established by constructing a suitable auxiliary function.

2. We explore the mass loss or gelling phenomena together with nonexistence aspect of the solution for some specific aggregation rate of the discrete SDAE. More

specifically, we prove that for a specific growth rate of the aggregation kernel, the solution of the equation (1) is not mass conserving in any interval of time. We also prove that nonexistence of any non trivial solution as consequence of the instantaneous gelling result.

3. To achieve the steady state from the pure aggregation equation, we introduce a extension of the discrete SDAE with some external physical condition. In particular, we consider the discrete Safronov-Dubovskiĭ aggregation equation with two external physical condition. These external forcing terms help us to balance the particle size in the system and to achieve the stationary state of the system. For the theoretical establishment of the considered model, a complete mathematical investigation for well-posedness to the discrete SDAEWF model has been covered in this study.

4. We establish the existence of unique equilibrium solution of the discrete SDAEWF model for a suitable restriction on the forcing coefficients. Moreover, we also prove that any solution to our considered model converges to the equilibrium solution with exponential rate of convergence.

6 REFERENCES

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Das, A. and **J. Saha** (2023) Trend to equilibrium solution for the discrete safronov–dubovskiĭ aggregation equation with forcing. *Proceedings of the Royal Society of Edinburgh: Section A Mathematics*, 1–24. URL: https://doi.org/10.1017/prm.2023.116.

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7 PROPOSED CONTENTS OF THE THESIS

8 LIST OF PUBLICATIONS BASED ON THE RESEARCH WORK

Refereed Journals

1. **Arijit Das** and Jitraj Saha, (2021). On the global solutions of discrete Safronov-Dubovskiĭ aggregation equation. *Zeitschrift für angewandte Mathematik und Physik*, **72**(5), 1–17.
   URL: https://doi.org/10.1007/s00033-021-01612-9

2. **Arijit Das** and Jitraj Saha, (2022). The discrete Safronov-Dubovskiĭ aggregation equation: Instantaneous gelation and nonexistence theorem. *Journal of Mathematical Analysis and Applications*, **514**(1), 126310.
   URL: https://doi.org/10.1016/j.jmaa.2022.126310

3. **Arijit Das** and Jitraj Saha, (2023). Trend to equilibrium solution for the discrete Safronov-Dubovskiĭ aggregation equation with forcing. *Proceedings of the Royal Society of Edinburgh Section A: Mathematics*, 1–24
   URL: https://doi.org/10.1017/prm.2023.116

International Conferences

1. **Arijit Das** and Jitraj Saha: 1^{st} *International Conference on Applied Analysis, Computation and Mathematical Modeling in Engineering*, Feb 24-26, 2021, Department of Mathematics, National Institute of Technology, Rourkela, India.
   URL: https://doi.org/10.1007/978-981-19-1824-7

2. **Arijit Das** and Jitraj Saha: 36^{th} *Annual Conference of Ramanujan Mathematical Society*, Aug 5-7, 2021, Department of Mathematics, Amrita School of Engineering Amrita Viswa Vidyapeetham, Coimbatore.
   URL: https://doi.org/10.1007/s41478-022-00407-z