SYNOPSIS OF

NUMERICAL SOLUTION OF NON-LINEAR PARTICULATE MODELS

A THESIS
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1 INTRODUCTION

The interactions among the particles suspended in a fluid medium or interacting with each other in a particulate system lead towards the change in particle population and their physical properties. This phenomena is coined as particulate processes. The application of these processes can be found widely, ranging from naturally occuring events to different controlled laboratory/manufacturing units. They provide a deeper understanding and insight of natural and industrial process such as crystallization, granulation [Ismail et al. (2020); Szulc et al. (2024)], polymerization [Costa et al. (2007); Pohar and Likozar (2014)], precipitation [Di Veroli and Rigopoulos (2010); Hoffmann and Feingold (2023)], multiphase flow and reaction [Yeoh et al. (2013); Rowe and Yates (2020)], astrophysics and astronomy [Ramkrishna and Singh (2014); Mishra and Sana (2021)], pharmaceutical [Mangin et al. (2006); Lahiq and Alshahrani (2023)] etc.

Significant practical implications of particulate models encourages the scientific community for extensive examination of the underlying physics which lays a foundation for modeling and optimization of these processes. The primary physical mechanisms includes aggregation, breakage, growth, nucleation and diffusion. These processes involve different physical laws and interactions. We now briefly explain these particulate process. When particles combine or aggregate to form a larger particle, is referred as aggregation or coagulation. On the other hand, breakage describes the opposite phenomena, where particle disintegrates to form smaller ones due to some external force or collision among the fellow particles. Moreover, growth in particle's size or volume is the result of accumulation of non-particulate matter on particle's surface and nucleation occurs as a consequence of the condensation of non-particulate materials. During aggregation, breakage and nucleation process the number of particles in the system evolve with time, however it remains unchanged during growth. In addition to these processes, some external factors may influence the evolution of particle population in the system. The notion of source term is used to represent these factors. Thus new particles can either be introduced to the system or can be removed or it can be any other event which have an immediate effect on particle population.

The dynamic evolution of particle population within a system is described using a fundamental mathematical framework popularly known as population balance equation (PBE). In general, PBEs are integro-partial differential equations supported by some initial data. Details of these PBEs can be referred from

[Ramkrishna (2000)]. We now formally present the PBE describing simultaneous aggregation, linear breakage, growth, nucleation and source factors in defined by [O'Sullivan and Rigopoulos (2022)] as

$$\begin{aligned}\frac{\partial n(x,t)}{\partial t}+\frac{\partial[G(x,t)n(x,t)]}{\partial x} =&\frac{1}{2}\int_0^x \mathscr{A}(x-y,y)n(x-y,t)n(y,t)\mathrm{d}y-\int_0^\infty \mathscr{A}(x,y)n(y,t)n(x,t)\mathrm{d}y\\ &+\int_x^\infty b(x|y)S(y)n(y,t)\mathrm{d}y-S(x)n(x,t)+N(x)+B_{src}(x,t),\end{aligned} \tag{1}$$

associated with the initial condition

$$n(x,0)\geq 0, \quad \text{for all} \quad x\geq 0. \tag{2}$$

The first term on the left hand side of the equation (1) is the time evolution of the particle density $n(x,t)$ of x (≥ 0) size particles at time t (≥ 0). The second term on left defines growth process and $G(x,t)$ is the rate of particle growth. The first two terms on the right hand side describe the aggregation process. The kernel $\mathscr{A}(x,y)$ is the aggregation rate at which particles of size $x+y$ are forming due to accumulation of x and y size particles. In general, it is assumed that $\mathscr{A}$ is positive and symmetric with respect to its arguments. The third and fourth terms are due to breakage, where $S(y)$ is the selection function which gives the rate at which particle of size y are selected to break and $b(x|y)$ is breakage function which gives the distribution of daughter particle x which are formed due to breakage of mother particle y. Since, the external force induces this breakup so it is a linear model. Fifth term $N(x)$ describes nucleation of particles and the last term $B_{src}(x,t)$ is the source term.

Literature reports particle breakage due to collision of two particles. It is referred as collisional or collision-induced breakage since two particles are involved in breakup process, Hence its is a non-linear model. The mathematical representation of this type of breakage is given by [Cheng and Redner (1988, 1990)]

$$\begin{aligned}\frac{\partial n(x,t)}{\partial t}=&\int_0^\infty\int_x^\infty \mathscr{B}(x|y;z)\,\mathscr{K}(y,z)\,n(y,t)\,n(z,t)\,\mathrm{d}y\mathrm{d}z\\ &-\int_0^\infty \mathscr{K}(x,y)\,n(x,t)\,n(y,t)\,\mathrm{d}y,\end{aligned} \tag{3}$$

with initial data (2). The collision kernel $\mathscr{K}(x,y)$ in equation (3) describes collision rate between particles of size x and y. Like the aggregation kernel, collision kernel $\mathscr{K}(x,y)$ is also a symmetric, non-negative function. The breakage kernel $\mathscr{B}(x|y,z)$

denotes the distribution of daughter particle of size x, which are fragmented from the particle of size y due to its impact with a particle of size z.

Apart from the particle density function, its integral moments are of utmost importance due to their physical significance. Let $\mathscr{M}_i(t)$ denotes the i^{th} moment and is defined as

$$\mathscr{M}_i(t) = \int_0^\infty x^i n(x,t)\mathrm{d}x. \tag{4}$$

The zeroth moment $\mathscr{M}_0(t)$ gives the total number and the first moment $\mathscr{M}_1(t)$ corresponds to the total mass of the particles present in the system.

2 MOTIVATION

This thesis has two-fold motivation, which evolves on two key aspects: models and methodology. They not only define the scope of the work but also serve as the pillars upon which the content of this thesis is built. To provide a clear perspective, we first outline the motivation for each aspect individually and then interlink the ideas to present a coherent and comprehensive framework for this research.

(i) Model-based motivation: Due to the wide scope and applications of PBEs, many researchers have attempted to model the system mathematically and solving them analytically or numerically. Note that most of the concentration lies on solving individual processes. From the application point of view, simultaneous process occur in various fields such as soot formation, bubble column, crystallization, cheese production etc [Bhole et al. (2008); Fox et al. (2017); Liu and Rigopoulos (2019); O'Sullivan and Rigopoulos (2022)]. Among all the particulate processes in equation (1), aggregation is nonlinear in nature. Consequently, other particulate model exhibit a significant degree of complexity and non-linearity in particular when coupled with aggregation. Exact solutions are available for a limited class of simple kernels. Since, aggregation involves convolution term, therefore transformations like Laplace, Mellin etc. are extensively used to solve such models for exact solutions. However, problem becomes challenging in the absence of convolution terms, which are infused in the model due to the coupling of with particulate process other than aggregation (refer to equation (1) and (3)). Therefore, numerical methods are generally employed to estimate the solutions in order to gain better insights of such systems.

Note that among certain popular particulate models, collisional breakage model is least explored as compared to the linear counterpart as it is highly non-linear and unlike aggregation, does not have convolution term. Hence, analytical solutions are only available for a very limited and particular combinations of collision kernels and breakage rates [Kostoglou and Karabelas (2000); Vigil et al. (2006); Ernst and Pagonabarraga (2007)], some scaling solutions are studied in [Cheng and Redner (1990)]. Existence and uniqueness of solution for the continuous collisional breakage equation is studied recently in [Paul and Kumar (2018); Giri and Laurençot (2021); Das and Saha (2022, 2024)] for a certain large class of kernels. There are only few studies which treat collisional breakage equation numerically [Das et al. (2020); Das and Kumar (2021)]. The limited development of effective and reliable numerical approximation techniques represents a significant gap in research, which serves as a key motivation for this study.

(ii) Methodological motivation: In literature, several techniques such as method of characteristics, discrete element method, stochastic methods, method of moments, sectional methods, semi-analytical methods etc. are available to solve particulate models [Kostoglou and Karabelas (1995); Kumar and Ramkrishna (1997); Nicmanis and Hounslow (1998); Marchisio et al. (2003); Aamir et al. (2009); Irizarry (2012); Kumar et al. (2013); Singh et al. (2022)] and references therein. All the above methods claims to be very robust and versatile, and have been mostly used to deal with individual particulate process or a combination of any two of them. However, they have several unaddressed limitations. In most occasions they compromise either with accuracy or computational time.

In the recent years, as an alternative to the traditional approximation techniques, semi-analytical methods in particular homotopy analysis method (HAM) [Liao (2003)] has gained much popularity to solve real-life problems. So, for the first time we explore HAM for solving simultaneous PBEs. It is based on the idea of deforming a complex problem into an infinite number of linear sub-problems. The approximate solution to the original problem is then obtained by summing the solutions from the first few sub-problems. HAM combines the advantages of perturbation and numerical methods and can be used to approximate solutions for a wider range of non-linear problems. Other semi-analytical methods such as homotopy perturbation method (HPM) [Kaur et al. (2019)], Adomian decomposition method (ADM) [Singh et al. (2015)] are the special cases of HAM.

The motivation for using section methods lies in their ability balance efficiency, flexibility and accuracy while dealing with complex particulate models. While other methods struggle with high computational cost or fails to capture the integral properties of particle distribution, section methods overcome these limitations. These methods are employed by discretizing the size domain into finite sub-intervals or cells. All the cell properties are assumed to be concentrated at a cell representative called pivots (mostly at the midpoint of each cells). Consequently, a set of ordinary differential equations is obtained to describe the variation in the number of particles using any numerical quadrature method. Thus, the continuous PBE is being replaced with an equivalent discrete equation. The scheme is designed in such a way that underlying particle properties are preserved exactly.

With the motivation outlined above, we begin by employing HAM to solve individual and simultaneous aggregation-fragmentation equation [put $G = N = B_{src} = 0$ in equation (1)]. This approach demonstrates the potential of homotopy based techniques to approximate the solution of such complex systems. While it generates highly accurate approximations and gives the solutions in closed form, it demands substantial computational time. Therefore, we change our attention to sectional methods to evaluate their performance in terms of both accuracy and computational cost. Moreover, it will be interesting to identify the particle processes or conditions on the system, for which a methodology proves to be the most efficient. This inspires the comparative study of numerical techniques, which is one of the major research gap in population balance studies. Furthermore, considering more than one particle property contributes to the complexity of the systems and hence makes it challenging to approximate their solutions. Solving multidimensional PBEs is a long-standing and intricate problem in the particulate sciences. This leads to the motivation of extending them to multidimensional models.

To address the collisional breakage equation numerically, we employ a series of sectional methods. We thoroughly examine the challenges in the implementation of each of these methods and develop strategies to overcome them. This enhances the overall accuracy and efficiency of the techniques while delivering cost effective solutions. The refinement and increased adaptability ensures the robustness of proposed methods. We identify the most effective section-based methodology for collisional breakage model by evaluating the performance of each approach by comparing them. Moreover, we extend the technique which generates most accurate solutions to solve multidimensional model.

3 OBJECTIVES AND SCOPE

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

(i) Aggregation and breakage are two of the most occurring phenomena of particulate process and hold great physical significance. We aim to solve them individually and the coupled process using HAM. This work establishes the foundation of semi-analytical approaches for solving PBEs. We consider a wide range of empirical kernels and analyse the solution behaviour. Along with this, convergence analysis of the recursive scheme proves that the series solution will eventually converge to the exact solution.

(ii) Note that a number of particulate events are responsible for the particle evolution dynamics in population balance systems. Their effects will be studied through a number of examples and are validated against existing sectional methods. This approach will identify the strengths and limitations of the numerical techniques. Both semi-analytical and sectional methodologies will be further extended to solve multidimensional models. This can be considered as a comprehensive study on various solution techniques for solving simultaneous PBEs. Therefore, it will be beneficial for the researchers working in industry and CFD modeling to identify the best method according to their requirements.

(iii) Collisional breakage equation is challenging to deal with on account of non-linearity and two integrals appearing in the birth term. We propose two section based approaches, where the birth term is modified in order to conserve the total number of particles and total mass of the system. These interesting approaches differ in terms of allocating the daughter particles born in a cell to the neighbouring pivots. Based upon the system's requirement these methodologies can implemented which optimizes the performance of the system.

(iv) We propose another numerical treatment of collisional breakage equation which differs completely from the above mentioned approaches. In this approach, first the average of particle property is calculated and then the birth of all the particle in a cell is assigned to the neighbouring cells. Here, three cells participate in the particle allocation, which will greatly enhance the accuracy of the numerical scheme in predicting the solution. Moreover, the multidimensional extension will give improved insights of the systems mechanism and bhevaiour.

4 DESCRIPTION OF THE RESEARCH WORK

4.1 Homotopy analysis method

The thesis focuses on the numerical treatment of various particulate processes. We start with the formulation of a numerical scheme based on the homotopy analysis method to solve aggregation breakage models including the simultaneous event is discussed. We consider several test cases and analyze them qualitatively and quantitatively to ascertain the improved accuracy and efficiency over the existing semi-analytical models. For some test cases, we obtain the generalized solution of the problem which converges to exact solution in limiting sense. We also study the detailed convergence analysis of the scheme.

4.2 Performance analysis of semi-analytical and sectional methods

This portion of the thesis is devoted to the comparative study of semi-analytical and section method. We consider simultaneous PBE incorporating diverse particulate process aggregation, breakage, growth, nucleation and source. Finding analytical solution is quite challenging for this equation due to the complex and non-linear nature, and it involves kinetic rates for each process. We solve simultaneous PBEs using sectional and semi-analytical technique. We discuss the performance, adaptability and accuracy of both the methods in detail. We introduce the iterative scheme for semi-analytical method and perform convergence analysis using Banach fixed point theorem.

4.3 Fixed pivot techniques for collisional breakage equation

In this part of the thesis, we consider collisional brekage equation and approximate its solution based on descretization techniques. This study is carried out in two parts. In the first one, we obtain the scheme by modifying the birth of the discretized equation. It is done by allocating the new born daughter particles to their neighbouring cells. This plays a vital role in efficiency of the proposed model as it ensures the preservation of particle properties. We also introduce a new finite volume scheme for collisional breakage equation to validate the results of new scheme. We conduct the numerical validation through several examples, which shows that the scheme predicts number density with high accuracy and is consistent with moments. Moreover, we obtain first order convergence over uniform, non-uniform grids through experimental order of convergence. In the second part of the study, we first revise the continuous equation by modifying the birth term according to the size of the daughter particles post breakup event. The revised equation is then discretized using mean value theorem. This proposed scheme preserves two fundamental integral properties of number density with any specific measures. Interestingly, we observed that this scheme is second order accurate over a wide range of grid types. We validated the numerical findings of this approach with scheme introduced earlier. This technique produced highly efficient results for particle properties.

4.4 Cell average technique for collisional breakage equation

In this technique, we propose a different modification strategy for birth term. Here, the newly born particles are allocated to three adjacent cells depending upon their average value in each cell. The solutions obtained by pivot techniques becomes inconsistent over random grids. This modification not only improves the numerical model by making it consistent over random grids but also enhances the accuracy. In addition, we have also identified the conditions upon kernels for which the convergence rate increases significantly and achieves second order of convergence over uniform, non-uniform, locally uniform and random grids.

4.5 Multidimensional extension of collisional breakage equation

The approach based on cell average performed the best in terms of accuracy and consistency. Motivated from the success of the cell average technique, we extend it to solve multidimensional collisional breakage equation. We modify the birth term in such a way that four particle properties are preserved exactly. The results are compared the exact quantities available in literature.

5 CONCLUSIONS

We list out the following conclusions.

1. We employ HAM to solve aggregation breakage equation. The method generates series solution and corresponding recursive scheme for the same is obtained. We performed convergence analysis for the scheme. The comparative study is executed with respect to and homotopy perturbation method (HPM). In several instances, existing methodology fails to predict the moments, however HPM predicts them with high accuracy. The rigorous error analysis supports this claim. We observe that results from HAM-based solutions exhibit better agreement with analytical solutions as compared

to HPM. Furthermore, HPM genrates poor results as the size dependency of the model increases.

2. We conduct a comparative study to evaluate the performance of numerical techniques for solving simultaneous PBEs incorporating various particulate processes. The numerical techniques includes well known sectional method (cell averaging technique or CAT) and semi-analytical methods (HAM and HPM). We consider several physics-embedded test cases to validate the numerical solutions obtained from HAM, HPM and CAT. The HAM's ability to achieve satisfactory results with a limited number of terms in the series solution demonstrates its accuracy in predicting key properties. In addition, HAM outperforms CAT and HPM in terms of reliability and accuracy whereas CAT is cost effective.

3. We introduce two new sectional methods to approximate the solution of the nonlinear collisional population balance breakage equation. Both the approaches are robust and adaptable based on the system's requirement. In first approach the discretized birth term is modified whilst in the second one modification in the continuous term is performed. Both the schemes generates excellent results and are consistent with zeroth and first order moment.

4. We establish one more section based scheme, where the average of particle property in a cell plays the crucial role in allocating the particles in neighbouring cells. This scheme is second order convergent over different grids type including random ones. It not only preserves first two moments but also generates highly efficient results for higher order moments. Out of all the presented schemes, this one outperforms each one them.

5. We extend cell average technique for two dimensional collisional breakage equation. the discretization is performed over rectangular grids. The scheme is inline with prechosen particle properties.

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8 LIST OF PUBLICATIONS BASED ON THE RESEARCH WORK

Refereed Journals

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1. Prakrati Kushwah and Jitraj Saha: 1^{st} International Conference on Latest Advances in Computational and Applied Mathematics, February 21 -24, 2024, Department of Mathematics, Indian Institute of Science Education and Research Thiruvananthapuram, Kerala, India.

2. Prakrati Kushwah and Jitraj Saha: 4^{th} International Conference on Frontiers in Industrial and Applied Mathematics , December 21-22, 2021, Department of Mathematics, Sant Longowal Institute of Engineering & Technology, Longowal, Punjab, India.