ANALYSIS OF GAS-PARTICLE FLOWS THROUGH
MULTI-SCALE SIMULATIONS

Yile Gu

A DISSERTATION
PRESENTED TO THE FACULTY
OF PRINCETON UNIVERSITY
IN CANDIDACY FOR THE DEGREE
OF DOCTOR OF PHILOSOPHY

RECOMMENDED FOR ACCEPTANCE
BY THE DEPARTMENT OF
CHEMICAL AND BIOLOGICAL ENGINEERING
ADVISER: PROF. SANKARAN SUNDARESAN

JANUARY 2018
Abstract

Multi-scale structures are inherent in gas-solid flows, which render the modeling efforts challenging. On one hand, detailed simulations where the fine structures are resolved and particle properties can be directly specified can account for complex flow behaviors, but they are too computationally expensive to apply for larger systems. On the other hand, coarse-grained simulations demand much less computations but they necessitate constitutive models which are often not readily available for given particle properties. The present study focuses on addressing this issue, as it seeks to provide a general framework through which one can obtain the required constitutive models from detailed simulations.

To demonstrate the viability of this general framework in which closures can be proposed for different particle properties, we focus on the van der Waals force of interaction between particles. We start with Computational Fluid Dynamics (CFD) - Discrete Element Method (DEM) simulations where the fine structures are resolved and van der Waals force between particles can be directly specified, and obtain closures for stress and drag that are required for coarse-grained simulations. Specifically, we develop a new cohesion model that appropriately accounts for van der Waals force between particles to be used for CFD-DEM simulations. We then validate this cohesion model and the CFD-DEM approach by showing that it can qualitatively capture experimental results where the addition of small particles to gas-fluidization reduces bubble sizes. Based on the DEM and CFD-DEM simulation results, we propose stress models that account for the van der Waals force between particles. Finally, we apply machine learning, specifically neural networks, to obtain a drag model that captures the effects from fine structures and interparticle cohesion. We show that this novel approach using neural networks, which can be readily applied for other closures other than drag here, can take advantage of the large amount of data generated from simulations, and therefore offer superior modeling performance over traditional approaches.
I consider myself very lucky to have been advised by Professor Sundaresan. For the past 5 years, I appreciate that he has not only given me guidance, but also has taken much time to explain the reasons behind it. From our meetings, email exchanges, and his patient edits of my writings, I have learned from him how to think in a systematic manner and clearly express one's thoughts. There essential skills would otherwise have been difficult to develop. In one’s PhD study, there are invariably difficult times. For me, these difficult times have been made much easier to endure because I know that Sundar would always be there for me and do what he best can to help me. I am very grateful to it.

Besides Professor Sundaresan as my principal research mentor, I have received great mentorship from post-doc/senior graduate student throughout my PhD study. First and foremost, Ali Ozel has been instrumental in many of the works in this thesis. He always puts others ahead of himself, and I am so glad that he is now Professor Ozel, a title he truly deserves. Shortly after I joined the lab, Sebastian Chialvo took time out of his busy schedule (as he tried to finish his thesis) to show me how to conduct computational research, which laid a strong foundation for my later studies. In the later stage of my PhD study, I feel so fortunate to have Jari Kolehmainen join our lab. He always patiently listens to my problems in research, and much to my amazement can consistently come up with valuable insights.

I want to thank my committee members: Professor Kevrekidis, Professor Mueller, and Professor Brun. I want to specifically thank Professor Kevrekidis for introducing me to machine learning. I still can remember the moment of my excitement when he talked about eigenfaces in his lecture. I also want to thank Karen Oliver for her help throughout my time in Princeton. Her kindness to people around her is something I would always remember and try to emulate.
My research group has been nothing but amazing. I feel that my lab is the Scranton branch in the American TV show *the Office*: a very close-knit community. We not only work in the same office, but also do fun things together outside the office. Aside from Ali, Sebastian, and Jari, I have greatly enjoyed my time with Greg Rubinstein. We share many interests: NBA, the TV show *the Office*, and many others, which we often chat about when we take a break from research. Matt Girardi has been my deskmate, and I always enjoy our conversations ranged from research to some random thing read off the internet. I have enjoyed taking trips with Chris Boyce in Utah and California after we attended conferences; they were truly great times. I also spent a memorable summer when Yushan Zhang was a summer intern in our lab. Together with other friends, we went to a shooting range and also did fine dining in New York City, which were both new to me. That summer was the best summer in Princeton. Throughout my time at lab, I have also had a chance to interact with many other lab members who hail from many parts of the world: Shuyan Wang, Lichao Cai, Chris Milioli, Fernando Milioli, Ziv Greidinger, Sia Darvishmanesh, Wendy Jiang, and Xiaoyu Liu. They have all enhanced my experience at Princeton.

I am blessed to be surrounded by many friends while at Princeton. I am especially grateful for having a very close circle of lifelong friends: Will Mulhearn, Yogesh Goyal, Dmitry Pozharskiy, Tom Bertalan, and Alexander Holiday. We have spent numerous nights playing board games, celebrated each other’s birthday, travelled around the world, and done many other things together. What I appreciate the most about this friendship, which in my opinion could be just important as this dissertation, is that we deeply understand each other, and that I can be myself without worries.

When I am tired from studies and research, I often find myself watching the TV show *the Office*. In many ways, these fictional characters, Jim, Dwight, Michael, Pam and others, have had an impact on me just as much as the real people. They have not only brought immense joy to me, but also taught me so much about life. I have learned the importance of
being true to myself and living the life to the fullest. As Pam said in the finale, “There’s a lot of beauty in ordinary things.” This saying truly resonated with me, and I tried to remember it as I went through my life in Princeton to remind myself to appreciate the little things happening around me. As I watch the Office again and again, Scranton becomes Princeton, and Princeton becomes Scranton.

I want to thank my parents, Zhou Gu and Shuqin Yang. In many ways, this dissertation is just as important to me as to them, and this dissertation is just as much about my endeavors as about their endeavors. Ever since I was born, they have devoted their lives on me to ensure that I would have a best education possible. Their entire lives revolve around me, even today as we live on the opposite sides of the world. I hope this dissertation which symbolizes the fruition of my education would in a humble way serve as a testament to their tremendous commitment to me. I feel honored to be able to dedicate this dissertation to them.

Finally, I would like to acknowledge the funding sources of my thesis work. This work is made possible by fundings from the Department of Energy and ExxonMobil Res. & Eng. Co., as well as Charlotte Elizabeth Procter Honorific Fellowship from Princeton University.
Scholarly Presentations and Publications

This thesis contains work that has been published, submitted, or in preparation for publication in peer-reviewed journals. Those works are listed below:


This thesis also contains work that has been presented at professional conferences. Those works are listed below:


To my parents, Shuqin Yang and Zhou Gu, for their profound love.
Contents

Abstract ................................................................. iii

Acknowledgements ....................................................... iv

1 Introduction  .......................................................... 7

1.1 Gas-particle flows and simulation approaches ...................... 7

1.2 Scope of investigation ............................................. 12

2 Rheology of cohesive and polydisperse granular materials across dense-flow regimes  .................................................. 17

2.1 Simulation methodology .......................................... 18

2.2 Rheology of cohesive granular materials  ......................... 22

2.2.1 Introduction ...................................................... 22

2.2.2 Flow regimes .................................................... 23

2.2.3 Pressure .......................................................... 29

2.2.4 Shear stress ratio .............................................. 33
2.2.5 Generality of the results ........................................... 36
2.2.6 Conclusions ......................................................... 41

2.3 Rheology of granular materials with particle size distributions. ........... 42
   2.3.1 Introduction .................................................... 42
   2.3.2 Particle size distributions .................................. 43
   2.3.3 Flow regimes .................................................... 45
   2.3.4 Pressure .......................................................... 47
   2.3.5 Shear stress ratio .............................................. 55
   2.3.6 Conclusions .................................................... 57

3 Development and validation of CFD-DEM approach for cohesive particles 60
   3.1 Development of a modified cohesion model to be used in CFD-DEM simulations 62
      3.1.1 Introduction .................................................... 62
      3.1.2 Simulation methodology .................................... 63
      3.1.3 Simulation conditions ...................................... 68
      3.1.4 Results and discussions .................................... 71
      3.1.5 Conclusions .................................................... 88
   3.2 Investigation into the effects of fines on fluidization through CFD-DEM simulations 91
      3.2.1 Introduction .................................................... 91
3.2.2 Simulation conditions .............................................. 94
3.2.3 Results and discussions ........................................... 100
3.2.4 Conclusions ......................................................... 110

4 Rheology of non-cohesive and cohesive granular materials in gas-fluidized suspensions ....................................................... 112

4.1 Introduction .............................................................. 113
4.2 Simulation conditions ................................................. 115
4.3 Simulation results ...................................................... 116
  4.3.1 Non-cohesive particles .......................................... 120
  4.3.2 Cohesive particles ............................................... 131
4.4 Conclusions .............................................................. 143

5 Neural networks for drag modeling ...................................... 145

5.1 Introduction .............................................................. 146
5.2 Methodology ............................................................. 148
  5.2.1 Multi-Layer Perceptron ......................................... 148
  5.2.2 Data sets ............................................................ 150
5.3 Results ................................................................. 152
5.4 Conclusions ............................................................. 157
6 Summary and suggestions for future work

6.1 Summary ................................................. 159

6.2 Suggestions for future work .......................... 161
List of Figures

1.1 Illustrations of different simulation approaches in literature. .................. 10
1.2 Geldart classification system. ................................................................. 13
1.3 Organization of the chapters in this thesis. ............................................... 14
2.1 Locally averaged velocity versus position in the direction of shear. ............ 25
2.2 Scaled pressure versus scaled shear rate for non-cohesive and cohesive particles. 26
2.3 The average coordination number versus scaled shear rate at various modified Bond numbers. ................................................................. 28
2.4 Scaled pressure vs scaled shear rate. .......................................................... 28
2.5 Collapse of pressure versus shear rate curves. .......................................... 31
2.6 Collapse of pressure for inertial and quasi-static regimes. .......................... 31
2.7 Rescaled pressure versus solid volume fraction in the cohesive regime ......... 32
2.8 Shear stress ratio versus scaled shear rate. .............................................. 33
2.9 Model performance for the corrected Rumpf’s formula that accounts for non-affine particle displacements. .................................................... 35
2.10 The average coordination number versus volume fraction in the cohesive regime. 36

2.11 Scaled pressure versus scaled shear rate. 37

2.12 Shear stress ratio versus scaled shear rate. 38

2.13 Collapse of pressure versus shear rate curves. 39

2.14 Illustrations of various PSD considered. 44

2.15 Scaled pressure versus scaled shear rate. 46

2.16 Transition of pressure fluctuations between inertial and quasistatic regimes. 47

2.17 Collapse of pressure versus shear rate curves. 49

2.18 Collapse of pressure versus shear rate curves. 50

2.19 The dependence of jamming volume fractions on polydispersity, skewness, and types of size distribution. 53

2.20 Scaled pressure from simulations vs. model predictions in the quasistatic regime. 55

2.21 Shear stress ratio versus inertial number; yield stress ratio determined for different particle size distributions. 58

3.1 Schematic of the original and modified cohesion models. 67

3.2 The computation domain and boundary conditions. 69

3.3 Snapshots of fluidization of non-cohesive particles for Hookean contact model. 72

3.4 Cumulative volume fraction of bubbles versus bubble diameter for both Hookean and Hertzian contacts. 73
3.5 Representative snapshots of fluidization of non-cohesive particles for Hertzian contact model .................................................. 73
3.6 Snapshots of fluidization of cohesive particles for Hookean contact model. . . 75
3.7 Cumulative volume fraction of bubbles versus bubble diameter for both Hookean and Hertzian contacts. ................................................. 76
3.8 Representative snapshots of fluidization of cohesive particles for Hertzian contact models. ................................................................. 76
3.9 Snapshots of fluidization of cohesive particles for Hookean contact model. . . 78
3.10 Effective restitution coefficients versus impact velocities. ............................. 79
3.11 Effective restitution coefficients versus impact velocities. ............................. 85
3.12 Configuration of the simulation on a collision between a particle and an agglomerate. ................................................................. 86
3.13 Distribution of steady-state particle velocities from the simulations. ............... 87
3.14 Dynamics of the scaled domain-averaged slip velocities for base and fine particles. 97
3.15 Scaled volume medium bubble diameter versus domain-averaged solid volume fraction. ................................................................. 98
3.16 Snapshots of the fluidized systems. ..................................................... 99
3.17 Cumulative volume fraction of bubbles collected from the snapshots. .......... 99
3.18 Volume medium scaled bubble diameter versus domain-averaged solid volume fraction. ................................................................. 101
3.19 Cumulative volume fraction of bubbles collected from the snapshots for various fines contents. .......................... 102

3.20 Volume medium scaled bubble diameter versus domain-averaged solid volume fraction. ........................................ 104

3.21 Solid volume fraction at the minimum bubbling condition for various fines contents found in experiments and present simulations. ............... 104

3.22 Volume medium scaled bubble diameter versus domain-averaged solid volume fraction. ........................................ 105

3.23 Snapshots of the fluidized systems of an increased domain size. .......... 105

3.24 Scaled particle phase pressure versus domain-averaged solid volume fraction. ......................................................... 106

3.25 Average coordination number for all particles and for base particles $Z_b$ versus domain-averaged solid volume fraction. ..................... 107

3.26 Effective restitution coefficient versus impact velocity. .................. 110

4.1 Snapshots of the particle volume fraction field in a periodic domain. ...... 118

4.2 Normal stress components scaled by trace of the stress vs solid volume fraction. 119

4.3 Dimensionless trace of stress tensor vs dimensionless rate of dilation. .... 121

4.4 Dimensionless pressure vs dimensionless granular temperature and rescaled pressure vs solid volume fraction .......................... 122

4.5 Dimensionless bulk viscosity vs dimensionless granular temperature and rescaled bulk viscosity vs solid volume fraction. ..................... 124

4.6 Dimensionless shear viscosity vs dimensionless granular temperature. .... 126
4.7 Rescaled shear viscosity vs solid volume fraction. 126
4.8 Dimensionless shear viscosity vs dimensionless granular temperature. 127
4.9 Dimensionless production rate of PTE by shear vs dimensionless granular temperature. 130
4.10 Rescaled rate of production of PTE by shear scaled vs solid volume fraction. 130
4.11 Dimensionless production rate of PTE by shear vs dimensionless granular temperature. 131
4.12 Dimensionless pressure vs dimensionless granular temperature. 134
4.13 Average coordination number vs dimensionless granular temperature. 135
4.14 Scaled pressure contributed from cohesion vs solid volume fraction. 135
4.15 Dimensionless shear stress vs dimensionless granular temperature. 139
4.16 Shear viscosity subtracted by the component corresponding for non-cohesive particles vs solid volume fraction. 139
4.17 Dimensionless rate of production of PTE by shear vs dimensionless granular temperature. 142
5.1 Two neural network architectures used in the study. 150
5.2 Parity plot for drag corrections. 153
5.3 Probability density function of relative error. 154
5.4 Probability density function of relative error on different sets of features. 156
List of Tables

1.1 Simulation approaches for gas-solid flows in literature. .......................... 8

2.1 Values of model constants .............................................................................. 29

3.1 Parameter values used in the simulations. ......................................................... 70

3.2 DEM time steps employed for simulations. ....................................................... 70

3.3 Scaled pressure versus scaled shear rate. ......................................................... 83

3.4 Summary of previous experimental investigations. ......................................... 93

3.5 Parameter values used in the simulations. ....................................................... 96

3.6 Effects of interparticle cohesion pairs on bubble size reductions. .................. 108

4.1 Computational domain and simulation parameters. ......................................... 117

4.2 Computationally generated kinetic-theory-based models for non-cohesive and cohesive particles proposed in the present study. ......................... 141

5.1 Pearson correlation coefficient between values from model predictions and actual values. .......................................................... 152
Chapter 1

Introduction

1.1 Gas-particle flows and simulation approaches

Gas-particle flows are found in a variety of chemical processing and energy conversion industries, where fluidized beds are utilized. These applications include catalytic cracking [1], coal combustion and gasification [2], coking [3], methanol-to-olefin production [4], chemical looping combustion [5], biomass gasification [6], carbon sequestration [7], etc. In spite of the prevalence of gas-particle flows in these industries, the scale-up and design of fluidized beds remains a challenge due to the complexity of flow behaviors. For example, gas-particle flows exhibit clustering phenomena that decrease the external surface area between solid and fluid phases, which results in decreased mass and heat transport [8]. Moreover, the solid particles in these systems have a wide range of shapes, sizes, densities, and other physical properties (e.g. particle-particle cohesion), which would further affect the overall flow behaviors of the systems [9]. As a result of the interplay of these complex phenomena, the scale-up of fluidized beds from laboratory scale to industrial scale is still based on extensive experimentation at several different intermediate scales [10]. Because of the time commitment, potential risk, and expense associated with pilot scale experiments, it is of much interest to develop de-
Table 1.1: Simulation approaches for gas-solid flows in literature.

<table>
<thead>
<tr>
<th>Simulation Approach</th>
<th>Advantages</th>
<th>Disadvantages</th>
<th>Usage</th>
</tr>
</thead>
<tbody>
<tr>
<td>PR-DNS (Particle-Resolved Direct Numerical Simulation)</td>
<td>Provide very accurate results.</td>
<td>Very small systems (typically &lt; 10,000 particles)</td>
<td>To develop constitutive models that describe fluid-particle interactions</td>
</tr>
<tr>
<td>CFD-DEM (Computational Fluid Dynamics - Discrete Element Method)</td>
<td>(1) Can simulate systems larger than PR-DNS. (2) Easily account for particle properties.</td>
<td>Cannot simulate industrial-scale systems.</td>
<td>(1) To simulate laboratory-scale experiments (2) To develop coarse-grained constitutive models</td>
</tr>
<tr>
<td>TFM (Two-Fluid Model)</td>
<td>Can simulate systems even larger than CFD-DEM.</td>
<td>(1) Cannot simulate industrial-scale systems. (2) Cannot easily account for different particle properties, which require closures.</td>
<td>(1) To simulate laboratory-scale experiments (2) To develop coarse-grained constitutive models</td>
</tr>
<tr>
<td>Filtered TFM</td>
<td>Can simulate industrial-scale systems.</td>
<td>Cannot easily account for different particle properties, which require closures.</td>
<td>To simulate industrial-scale systems.</td>
</tr>
<tr>
<td>Filtered MP-PIC (Multi-Phase Particle-In-Cell)</td>
<td>Can simulate industrial-scale systems.</td>
<td>Cannot easily account for different particle properties, which require closures.</td>
<td>To simulate industrial-scale systems. Less computationally expensive than filtered TFM for systems of particles with different properties.</td>
</tr>
</tbody>
</table>
velop appropriate computational tools that would enable simulations of fluidized beds at various scales. These computational simulations would enable better design and analysis of pilot scale experiments, and cut down the total cost and time to develop commercial scale processes. Furthermore, once the full-scale fluidized bed is built, these simulations can also assist in troubleshooting and optimizations during operations.

Due to the complexity of inhomogeneous structures present in gas-particle flows at various scales, different simulation approaches have been developed in the literature to model gas-particle flows at these different scales; each of these approaches has unique advantages and disadvantages. In the order of increasing scale, we discuss in the following several most commonly used simulation approaches in literature. They are summarized in Table 1.1, and their illustrations are provided in Figure 1.1.

In the first of these approaches, Newton’s equations of motion are solved for each particle, while the Navier-Stokes are solved for the fluid. Since that the fluid grid size is much smaller than the size of a particle, the two phases are coupled by enforcing a no-slip boundary condition along the particle surface [11]. This approach, known as Particle-Resolved Direct Numerical Simulation (PR-DNS), has advantages in that it provides accurate simulation results. Its disadvantage is that, due to computational limitations, it can only simulate systems with a small number of particles (typically < 10,000). Therefore, PR-DNS has been primarily used to develop constitutive models that describe gas-particle interactions (e.g. [12, 13]).

In the second of these approaches, known as CFD-DEM (Computational Fluid Dynamics - Discrete Element Method) [14], computational fluid phase is less resolved while Newton’s equations of motions are still solved for each particle. The dynamics of fluid phase is modeled by solving continuity and momentum equations discretized on grids of size equal to several particle diameters, and the interaction force between the fluid and particle is accounted for via a constitutive model. These constitutive models are typically obtained through
Figure 1.1: Illustrations of different simulation approaches in literature, in the order of increasing scale.

experiments or PR-DNS. CFD-DEM offers several advantages. Compared with PR-DNS, it can simulate larger systems with up to hundred million particles. It has been used to model many laboratory-scale experiments, and yields excellent agreement (e.g. [15, 16]). Furthermore, it can easily account for various particle properties, such as particle sizes (e.g. [17]) and complex particle-particle interactions (e.g. [17]). The major drawback of CFD-DEM is that, due to computational limitations, it cannot simulate industrial-scale beds where there are billions of particles.

The third approach is Two-Fluid Model (TFM) [18, 19]. In this approach, the fluid and particles are treated as interpenetrating phases. Continuity and momentum equations are solved for both fluid and solid phases. The grid size used is typically several particle diameters. This approach requires a constitutive model for the particle phase stress. Most of the simulations in literature employ kinetic theory of granular gases [18–23], which is a class of dynamic models developed to evaluate the transport coefficients by moment analysis of the Boltzmann equation. The earliest and most widely used kinetic theory models have been
analytically derived for dilute flows of inelastic, smooth, frictionless spheres with no effects from interstitial fluid [24–27]. These models have since been improved based on analyzing results from DEM simulations [28, 29]. The advantage of TFM approach is that it can be used to simulate relatively large systems (laboratory-scale) with fair accuracy (e.g. [16]), and typically with faster speed than CFD-DEM. The disadvantages are twofold. First, due to computational limitations, it cannot simulate industrial-scale beds. Second, it cannot easily account for complex particle-particle interactions, because of the need for a constitutive model for particle stress which has been mostly proposed for non-cohesive, monodisperse particles in literature.

The fourth approach is filtered TFM [30–34]. It is similar to standard TFM except for that the continuity and momentum equations are now solved on much larger grids. Agrawal et al. (2001) [35] found that TFM simulations with coarsened grids without properly accounting for fine-scale structures would yield unphysical results. A filtering approach has thus then been developed, in which fine-grid CFD-DEM or TFM simulations are used to develop filtered constitutive models for the fluid-particle interaction force and particle phase stress [30–32, 34, 36–39]. These filtered constitutive models are used to capture the effects of fine-scale structures, so that the simulations on coarsened grids with these closures would yield similar results as simulations on fine grids. The advantage of this approach is that it can simulate industrial-scale beds, and has shown good agreement with experimental data (e.g. [40]). The main disadvantage of the approach is that it is currently difficult to employ this approach in the presence of complex particle-particle interactions.

The fifth approach is filtered MP-PIC (Multi-Phase Particle-In-Cell) [41–46]. In this approach, similar to CFD-DEM, particles are solved in a Lagrangian fashion, but a smaller number of representative particles, named parcels, are tracked and particle-particle interaction is treated by tracking collisions between parcels [45, 46] or a physically reasonable particle phase stress model [41–44]. Fluid phase is still solved through continuity and mo-
mentum equations but on larger grids. Because of the coarse-graining for both phases, similar to filtered TFM, filtered constitutive models for fluid-particle interaction force that account for effects of fine-scale structures need to be employed [38, 47, 48]. The advantage of this approach is that, like filtered TFM, it can simulate industrial-scale beds. It has another attractive feature compared to filtered TFM. In filtered TFM, when the system has particles that possess different properties such as cohesion, friction, and size, particles with the same properties need to be treated as a separate phase. Correspondingly, additional continuity and momentum equations are needed for each new phase. Therefore, it would be computationally very expensive to simulate the system. In filtered MP-PIC approach, each parcel is a group of particles having same particle properties such as size, cohesion, friction, etc, which makes it much more computationally tractable. However, like filtered TFM, it suffers from the same issues of limited existing closures in literature for particle phase stress (if not tracking the particle collisions) and fluid-particle interaction force.

1.2 Scope of investigation

After reviewing these simulation approaches that exist in literature, one can readily see that all of these simulation approaches currently cannot be used to reliably simulate industrial-scale fluidized beds of particles with different properties (such as cohesion and size distribution). They are either limited to small system sizes (PR-DNS, CFD-DEM) or require constitutive models that only exist for particles with certain properties (e.g. non-cohesive and monodisperse in most cases) (filtered TFM/MP-PIC), or have both shortcomings (TFM).

This thesis focuses on addressing this issue, as it seeks to provide a general framework through which one can simulate industrial-scale fluidized beds of particles with any given property. In this general framework, one starts with a small-scale simulation such as PR-DNS or CFD-DEM where one can directly specify particle properties (such as cohesion,
size, shape), and then progressively coarse-grains the simulation results, and finally obtains constitutive models that are required for filtered TFM/MP-PIC. One can then run filtered TFM/MP-PIC with these closures that are “tailor-made” for these particle properties.

To demonstrate the viability of this general framework that can incorporate different particle properties, we focus on the van der Waals force of interaction between particles. It has been shown (e.g. [49]) that the van der Waals force of interaction between particles is responsible for the distinct flow behavior of Geldart Group A particles [9]. Group A particles are frequently encountered in industrial practices because that they are often easier to fluidize. In the Geldart classification system [9], particles are grouped in to groups A, B, C and D according to a combination of particle diameter $d_p$ and density difference between the solid and gas phase ($\rho_s - \rho_f$), as illustrated in Figure 1.2. Particles in each group exhibit similar fluidization characteristics: Group C particles are extremely cohesive and hard to fluidize; for Group A particles, uniform bed expansion is observed before bubbling occurs; for Group B particles, bubbles start to appear at or slightly above minimum fluidization velocity; Group D particles are spouted in fluidized beds.

Figure 1.2: Geldart classification system [9], reproduced from [50].
Therefore, this thesis aims to use van der Waals force of interaction as an example, to illustrate how one can obtain closures of filtered models for a given set of particle properties, which then can be used to run coarse-grid simulations. Closures for both drag and particle phase stress in the filtered model have been shown (e.g. [32]) to be important for predicting accurate flow behaviors. Thus, these two terms at various scales are the focus of the study here, as shown in Figure 1.3.

In Chapter 2, we propose a micro-scale continuum particle phase stress model that describes flow behavior at dense regime (at high solid volume fractions) using DEM-based simple shear simulations. Specifically, we study the effects of both van der Waals force and particle size distribution on particle phase stress. We find that the van der Waals force gives rise to a new flow regime where stress is shear rate independent. Introducing particle size distribution increases the jamming solid volume fraction in a systematic way that can be related to the distribution of particle size. In relation to the overall objective of thesis, this study provides a regime map for particle phase stress of cohesive particles. Also, one can use the stress model developed here to perform TFM simulations to develop filtered models.
In Chapter 3, we develop and validate the CFD-DEM approach that appropriately accounts for interparticle cohesion. In developing the CFD-DEM simulation approach, we propose a modified cohesion model to be used in the simulation. To speed up simulations, many studies in literature adopt small particle spring constants to allow for larger time steps. We show that this practice would yield unphysical results for cohesive particles. We then propose a modified cohesion model that is insensitive to particle spring constant. After developing this modified cohesion model to be used in CFD-DEM, we then apply the simulation approach to study a phenomenon that has puzzled many researchers and practitioners: the effects of fines on fluidization. Previous experiments have found that adding fines (particles with $d_p < 45 \mu m$) to fluidization would reduce bubble sizes. However, the mechanism is little understood. We show that the present CFD-DEM approach with the newly developed modified cohesion model can qualitatively capture this behavior, which then allows us to probe the underlying physics. Specifically, it is found that the interparticle van der Waals force of interaction is critical for the behavior. In relation to the overall objective of thesis, this chapter develops and validates a CFD-DEM approach that can account for inter-particle cohesion; as shown in Chapter 4 and 5, one can then run CFD-DEM simulations and post-process the results to develop stress models (Chapter 4) and drag models (Chapter 5) for filtered approach.

In Chapter 4, we develop a novel methodology through which one can develop micro-scale stress models for both non-cohesive and cohesive particles from analyzing results from CFD-DEM simulations. Compared with the stress model in Chapter 2, the developed model here has two advantages. First, it accounts for the effects of interstitial fluids. Second, it covers a wider range of parameter space. We first validate this methodology using non-cohesive particles, and show that it yields models that are consistent with the analytically derived kinetic theory. We then propose the stress models for cohesive particles. In relation to the overall objective of thesis, this chapter develops a novel methodology through which one can propose stress models for particles with complex inter-particle interactions. This stress
model can then be used in TFM simulations to develop filtered models. Alternatively, one can directly develop filtered stress models through CFD-DEM simulations.

In Chapter 5, we propose filtered drag models for both cohesive and non-cohesive particles. We first assume that van der Waals force does not affect the micro-scale drag (such as the model by Wen and Yu [51]) that is commonly used in CFD-DEM and TFM simulations. Although results not shown here, we have probed this assumption by running Lattice-Boltzmann simulations (PR-DNS) for non-cohesive and cohesive particles. It is found that similar drag coefficient is obtained between non-cohesive and cohesive particles. Therefore, in Chapter 5, we perform CFD-DEM simulations, and propose filtered drag models based on the simulation results. We apply neural networks in modeling, and demonstrate that they provide a substantial boost to model performance compared with traditional approaches. Specifically, we show that the trained neural network model, without retraining, can work reasonably well for particles with any particle size, cohesion level, and filter size. In relation to the overall thesis, the filtered drag model developed in this chapter can be directly used in filtered simulations.

In Chapter 6, we provide a summary over the main findings of this thesis. We also present some suggestions for future work. Specifically, in the light of the Chapter 5 which shows that neural networks can capture the filtered drag model substantially better than traditional approaches, we discuss about how to further utilize neural networks for problems in fluidization. Three general directions are suggested. First, one can apply neural networks to model other closures such as the particle phase stress. Second, one can utilize more complex neural network architectures to further improve the predicting power of the model. Third, one can look into how to best interpret the trained neural network model to help discover the underlying physics.
Chapter 2

Rheology of cohesive and polydisperse granular materials across dense-flow regimes

Overview of the chapter

We investigate the dense-flow rheology of granular materials with interparticle cohesion and particle size distributions (PSD) through DEM simulations of homogeneous, simple shear flows of frictional spherical particles. To study the effects of cohesion, different cohesion levels are added; to study the effects of size distributions, binary, linear, Gaussian, and lognormal distributions in size are considered. It is known [52] that dense shear flows of non-cohesive monodisperse granular materials exhibit three regimes: quasistatic, inertial, and intermediate. Stress is proportional to spring stiffness (and independent of shear rate) in the quasistatic regime; stress is proportional to square of shear rate (and independent of

spring stiffness) in the inertial regime; stress depends on both shear rate and spring stiffness in the intermediate regime. We study how this regime map as well as the the particle phase stress is changed with interparticle cohesion and particle size distributions:

- In the first part, we investigate rheology of cohesive granular materials. It is found that all the three regimes for non-cohesive particles (quasistatic, inertial, and intermediate) persist for cohesive granular materials. Cohesion results in bifurcation of the inertial regime into two regimes: (a) a new rate-independent regime and (b) an inertial regime, whose boundaries are determined by a modified Bond number, which is a ratio of cohesive force to a characteristic contact force. We propose a rheological model for cohesive systems that captures the simulation results across all four regimes.

- In the second part, we investigate rheology of granular materials with size distributions. It is found that all the regimes persist as well. However, the critical solid volume fraction that separates the quasistatic and inertial regimes is found to increase when particles manifest size distribution. This increase in the critical solid volume fraction can be predicted with fair accuracy by polydispersity and skewness alone regardless of types of distributions. Furthermore, the inertial number model for stress ratio is found valid for particles with size distribution. A rheological model is proposed that captures the simulation results on stresses for all the size distributions studied.

2.1 Simulation methodology

The DEM simulations [53] were performed using the molecular dynamics package LAMMPS [54]. Particles interact via repulsive spring-dashpot contact forces (and attractive cohesive forces for cohesive particles). In the spring-dashpot model, the normal and tangential contact forces on a spherical particle $i$ resulting from the contact of two spheres $i$ and $j$ with radii
\[ r_i \text{ and } r_j \text{ are} \]
\[ F_{n_{ij}} = f \left( \frac{\delta_{ij}r_i r_j}{r_i + r_j} \right) \left[ k_n \delta_{ij} n_{ij} - \gamma_n m_{\text{eff}} v_{n_{ij}} \right], \quad (2.1) \]
\[ F_{t_{ij}} = f \left( \frac{\delta_{ij}r_i r_j}{r_i + r_j} \right) \left[ -k_t u_{t_{ij}} - \gamma_t m_{\text{eff}} v_{t_{ij}} \right], \quad (2.2) \]

where \( \delta_{ij} \) is the overlap distance, \( k_n \) and \( k_t \) are spring elastic constants, \( \gamma_n \) and \( \gamma_t \) are viscous damping constants, \( m_{\text{eff}} = m_i m_j / (m_i + m_j) \) is the effective mass of spheres with masses \( m_i \) and \( m_j \), \( v_{n_{ij}} \) and \( v_{t_{ij}} \) are the normal and tangential components of relative particle velocity, and \( u_{t_{ij}} \) is the elastic shear displacement. For Hookean contact, \( f(x) = 1 \), while for Hertzian contact, \( f(x) = \sqrt{x} \). The magnitude of tangential force is limited by a static yield criterion, \( |F_{t_{ij}}| \leq \mu |F_{n_{ij}}| \), where \( \mu \) is the particle friction coefficient. We set values of \( k_t/k_n = 2/7 \) [55] and \( \gamma_t = 0 \). For convenience, a constant value for \( \gamma_n \) is used for all particles during the simulations. \( \gamma_n \) is chosen based on the effective mass of spheres \( (m_{\text{eff}}') \) for two identical particles with radii of 0.5. Specifically, for Hookean contact, \( \gamma_n \) is chosen such that the restitution coefficient \( e \equiv \exp \left( -\gamma_n \pi / \sqrt{4k_n / m_{\text{eff}} - \gamma_n^2} \right) \), where \( m_{\text{eff}} \) is now substituted by \( m_{\text{eff}}' \), would be equal to 0.7. For Hertzian contact, we employ the same value for \( \gamma_n / \sqrt{k_n / m_{\text{eff}}'} \), but now the restitution coefficient \( e \) depends on the collision velocities. For all the PSDs used in the simulations, all the particles have scaled radii smaller or equal to 0.5. Thus, as restitution coefficient \( e \) increases with decreasing \( m_{\text{eff}} \) for a given \( \gamma_n \), higher restitution coefficients would be obtained during the simulations than those specified for \( m_{\text{eff}}' \). It should be noted that the values for restitution coefficients have been shown to have insignificant on critical volume fractions [52], which justifies the usage of a constant \( \gamma_n \).

To account for cohesion, an attractive force \( F_{n_{ij}}^C \) is included so that the total normal force between the particles becomes \( F_{n_{ij}}^{T} = F_{n_{ij}} + F_{n_{ij}}^C \). For van der Waals force model, the cohesive
force between a pair of particles whose surfaces separated by a distance \( s \) is written as \([56]\)

\[
F_{n_{ij}}^C = -\frac{Ad^6}{6s^2(s + 2d)^2(s + d)^3},
\]

(2.3)

where \( A \) is the Hamaker constant. It is assumed that the force saturates at a minimum cutoff distance, \( s_{\text{min}} = \theta d \) \([56]\). Additionally, since the magnitude of the cohesive force decreases rapidly with separation distance, a maximum cutoff distance \( s_{\text{max}} = d/4 \) \([57]\) is used to accelerate the simulation process; for \( s > s_{\text{max}} \), cohesive force is neglected.

We also investigated the alternate model of Rognon et al. \([58]\),

\[
F_{n_{ij}}^C = -\sqrt{4k_nN_A\delta_{ij}},
\]

(2.4)

where \( N_A \) is specified as an input. Note that, in the static limit, where the relative particle velocity is zero, for Hookean contact, the total normal force between two particles is \( k_n\delta_{ij} - \sqrt{4k_nN_A\delta_{ij}} \). Accordingly, \(-N_A \) is the maximum attractive force between the two particles, experienced when \( \delta_{ij} = N_A/k_n \) \([58]\).

Differences between these two cohesion models are significant. The cohesive force in the van der Waals model (Eq. 2.3) is present before the particles collide and does not increase with overlap between particles. In Eq. 2.4, the cohesive force is only present when particles are in contact and increases with extent of overlap. Nevertheless, it will be seen that both models lead to qualitatively similar results, differing in quantitative details only modestly.

In the DEM simulations, assemblies of about 2000 particles (in study of cohesion) or 4000 particles (in the study of PSD) with density \( \rho_s \) and given distributions are placed in a periodic box with fixed volume \( V \). Through the Lees-Edwards boundary condition \([59]\), particles are subjected to homogeneous steady simple shear at a shear rate \( \dot{\gamma} \). The macroscopic stress
tensor is calculated as
\[
\sigma = \frac{1}{V} \sum_i \left[ \sum_{j \neq i} \frac{1}{2} r_{ij} F_{ij} + m_i (v'_i)(v'_i) \right],
\]  
(2.5)

where \( r_{ij} \) is the normal vector pointing from the center of particle \( j \) to that of particle \( i \), and \( v'_i \) is the fluctuating velocity of particle \( i \) relative to its mean streaming velocity. This stress tensor is further ensemble-averaged over many time steps. Ensemble-averaged pressure and shear stress can thus be obtained as \( p = (\sigma_{xx} + \sigma_{yy} + \sigma_{zz})/3 \) and \( \tau = \sigma_{xz} \). The stresses and shear rate are made dimensionless through scaling with effective diameter \( \bar{d} \), \( \rho_s \), and elasticity \( k = k_n \).

In the study of PSD, for the effective diameter \( \bar{d} \), several candidates are explored in this study: volume-averaged diameter \( d_{43} \equiv \frac{\sum_{i=1}^{N} d_i^4}{\sum_{i=1}^{N} d_i^3} \), Sauter-mean diameter \( d_{32} \equiv \frac{\sum_{i=1}^{N} d_i^3}{\sum_{i=1}^{N} d_i^2} \), and root-mean-cubed diameter \( d_{rmc} \equiv \sqrt[3]{\frac{\sum_{i=1}^{N} d_i^3}{N}} \), where \( N \) is the total number of particles. Volume-averaged diameter \( d_{43} \) is considered as it has been found suitable for \( \bar{d} \) for dense flows of binary mixtures [17, 60]. Furthermore, \( d_{43} \) is consistent with the mass-based particle interactions in the DEM modeling. Sauter-mean diameter \( d_{32} \) is considered as it has been often used to characterize flow behaviors of particles with PSD (e.g. drag law [61]). Root-mean-cubed diameter \( d_{rmc} \) is considered as it has been demonstrated a suitable diameter for dilute flow of mixtures [62]. Note that the dimensions of the spring constants and damping coefficients differ for Hookean and Hertzian contacts. Thus, for example, stress will be scaled using \( k/\bar{d} \) and \( k \) in Hookean and Hertzian contacts, respectively.

In the study of cohesion, as gravity is not included in the simulations, a modified Bond number \( Bo^* \) is introduced, which compares the maximum net cohesive force experienced by a particle to a characteristic contact force. For Hookean contact with the van der Waals force model, \( Bo^* = F_{coh}^{max}/(kd) \approx A/(24k\theta^2d^2) \), where \( F_{coh}^{max} \) denotes the maximum cohesive force. For Hertzian contact with the van der Waals force model, \( Bo^* = F_{coh}^{max}/(kd^2) \approx A/(24k\theta^2d^3) \). Simulation results indicate that the results are insensitive to the particular value for \( \theta \) (1.0 ×
10^{-5} \leq \theta \leq 4.0 \times 10^{-5}) for specified value of \( Bo^* \). For the results presented in the study here, \( \theta = 4 \times 10^{-5} \) is chosen [57]. For Hookean contact with the alternate cohesion model, \( Bo^* = N_A/(kd) \).

2.2 Rheology of cohesive granular materials

2.2.1 Introduction

For non-cohesive particles, three flow regimes have been identified – namely, the quasistatic, inertial, and intermediate regimes [52, 63–65] – each of which manifests different scalings of the mean stresses with shear rate and volume fraction. Numerous constitutive stress models have been constructed with these scalings in mind [52, 64, 66–71]. However, many granular flows involve cohesive interparticle forces for which the above models do not account. These cohesive effects are the primary focus of the present study.

Cohesion can result from a variety of sources – including van der Waals forces [72, 73], electrostatic forces [74], capillary forces [75], and solid bridges [76] – and has a strong impact on granular rheology. For example, agglomeration of particles has been observed in simulations of cohesive granular materials in various flow geometries [57, 58, 77–80]. Annular shear flow experiments [81] and plane shear simulations [57, 58, 82] have shown that cohesion increases the shear stress ratio \( \eta \), defined as the ratio of shear stress \( \tau \) to pressure \( p \). Both simulations and experiments have shown that the discharge flow rate from a hopper decreases with increasing cohesion [83]. Rotating-drum experiments reveal that cohesion increases avalanche size and leads to robust pattern formation on the surface [84–86]. Despite the number of such phenomenological studies, there is relatively little literature on constituting the rheological effects of cohesion. One notable work is that of Rognon et al. [58], which presents modifications to friction and dilatancy laws for non-cohesive particles to account for the
effects of cohesion observed in 2-D simulations. The present study goes beyond these earlier studies by exposing how the regime map for non-cohesive materials [52, 63–65] is altered by the introduction of cohesion and formulating explicit models for the mean stresses.

In the present study, we investigate the rheology of cohesive granular materials through discrete element method (DEM) simulations of homogeneous, simple shear flows of frictional and cohesive particles. Most of the simulations presented here are based on a linear (Hookean) spring-dashpot model [53] for particle-particle interaction and a commonly used model for van der Waals force between particles [56]. The quasistatic regime where the stress is proportional to spring stiffness (and independent of shear rate), the inertial regime where stress is proportional to square of shear rate (and independent of spring stiffness), and the intermediate regime where stress depends on both shear rate and spring stiffness – reported previously for non-cohesive particles [52] – persist even when cohesion is added. The presence of cohesion is found to introduce a new rate-independent regime where the stress depends on the strength of cohesion. These regimes persist when the Hookean contact model is replaced by a Hertzian contact model as well as when the van der Waals force model is replaced with an alternate cohesion model proposed by Rognon et al. [58], illustrating the robustness of these regimes. Finally, we also modify the blended stress model proposed by Chialvo et al. [52] for dense flows of non-cohesive particles to obtain an analogous model for dense flow of cohesive particles.

2.2.2 Flow regimes

We first consider Hookean contact and van der Waals cohesion. Simulations are performed for various shear rates, volume fractions, friction coefficients, and modified Bond numbers. Figure 2.2(a) plots the scaled pressure \( \frac{pd}{k} \) against the scaled shear rate \( \hat{\gamma} = \gamma d/\sqrt{k/(\rho_s d)} \) for non-cohesive particles with \( \mu = 0.1 \). Three regimes are present [52, 63–65]: quasistatic at low shear rates and high volume fractions, inertial at low shear rates and low volume fractions,
and intermediate at high shear rates and all volume fractions. The quasistatic and inertial regimes are separated by a critical volume fraction $\phi_c$ which is a function of $\mu$ as summarized in Table 2.1. When cohesive forces are included, however, it is found that this regime map is modified, as shown in Figures 2.2(b) and (c), where $Bo^*$ is $5 \times 10^{-6}$ and $5 \times 10^{-5}$ respectively. Some aspects remain unchanged: all three non-cohesive regimes persist with no change in $\phi_c(\mu)$, and the quasistatic and intermediate pressure values show no appreciable changes. However, the inertial regime is now bifurcated into two regimes occurring at different scaled shear rates: at higher $\hat{\gamma}$ the flow remains inertial (i.e. exhibiting Bagnold scaling), while at lower $\hat{\gamma}$ the flow becomes rate-independent. We term this latter, new regime the cohesive regime. As $Bo^*$ increases, this cohesive regime expands to encompass a larger domain of $\hat{\gamma}$, as illustrated in Figures 2.2(b) and (c).

In Figures 2.2, we present the results only from simulations in which the velocity profile in the statistical steady state is found to be linear indicating homogeneous shear. There is a conspicuous absence of simulation results in Figures 2.2(b) and (c) at the lower volume fractions and shear rates in the region representing transition from cohesive regime to inertial regime. In this region, the velocity profiles are found to be inhomogeneous. Figure 2.1 shows the scaled velocity profiles for two different scaled shear rates and domain-averaged volume fraction of 0.51. All other conditions are as in Figure 2.2(b). It is readily seen that a linear velocity profile was achieved for $\hat{\gamma} = 9.49 \times 10^{-4}$ (results included in Figure 2.2(b)), but not for $\hat{\gamma} = 3.16 \times 10^{-4}$ (and hence omitted from Figure 2.2(b)). It appears reasonable to hypothesize that the occurrence of an inhomogeneous state is a manifestation of shear-banding instability [87, 88] which has not been a focus of the present chapter. Chapter 4 explores this region further through analysis of results from CFD-DEM simulations, in which we observe a “dip” in the shear stress in this transition region, which has been shown to yield instability [89].
Figure 2.1: Locally averaged velocity versus position in the direction of shear. Domain-averaged volume fraction of particles is 0.51. Hookean contact and van der Waals force model are used with $\mu = 0.1$ and $Bo^* = 5 \times 10^{-6}$. $H$ denotes the thickness of the periodic box in the shear direction.

The cohesive regime corresponds well to previous results [57] which report the existence of a rate-independent regime due to cohesion. Also, the cohesive-to-inertial regime transition is in accord with results from dynamic shear cell experiments on slightly cohesive powders [81]; the pressure in these experiments is roughly rate-independent at low shear rates but increases significantly at higher shear rates. Finally, the impact of cohesion on the scaling of pressure with respect to shear rate is consistent with previous 2-D, constant-pressure shear simulations of Rognon et al. [58]. They utilize $NA/(pd)$ to characterize cohesion and find that, when $NA/(pd)$ is large, the solid fraction no longer varies with inertial number (defined by them as $\dot{\gamma} \sqrt{m/p}$ for particle mass $m$) in their dilatancy law, which corresponds to the rate-independent behavior we observe for the pressure in the cohesive regime. The present study details where this new rate-independent cohesive regime is located in parameter space with respect to the other three regimes and, for the first time, provides a comprehensive regime map for dense flows of cohesive granular materials capable of explaining all of the above behaviors.

Because previous works (e.g. [58, 90]) demonstrate the importance of microstructure on dense granular rheology, we aim to explain the cohesive-to-inertial regime transition in terms
of changes in microstructure. To this end, we study the average coordination number $Z$, which is defined as the average number of contacts per particle in the system. Specifically, $Z = 2n_c/n$, where $n_c$ is the total number of contacts (with particle overlap) and $n$ is the total number of particles in the system. When $\phi > \phi_c$, cohesion has negligible impact on $Z$ across all shear rates (i.e. quasistatic and intermediate regimes), as seen in Figure 2.3(a). For $\phi < \phi_c$, cohesion has a weak impact on $Z$ at high shear rates (i.e. inertial and intermediate regimes), but substantially increases the value of $Z$ in lower shear rate region (i.e. the cohesive regime), as seen in Figure 2.3(b). Thus, cohesion has an appreciable impact on $Z$ only in the cohesive regime, which is consistent with the pressure data shown in Figure 2.2.

To make this observation more transparent, we present in Figures 2.4(a) and 2.4(b) the variation of pressure with shear rate corresponding to conditions in Figures 2.3(a) and 2.3(b), respectively. It is clear that cohesion has only a weak impact on pressure (and, as presented later, shear stress) in quasistatic, inertial, and intermediate regimes. The emergence of rate-independent regime because of the cohesive force can be reasoned through the average coordination number $Z$ characterizing the microstructure. When a dense assembly of non-cohesive particles is subjected to steady (and slow) shear, jamming occurs at a critical volume fraction, $\phi_c$, which depends on the particle-particle coefficient of friction [90, 91] and there is a
corresponding average coordination number $Z_c$. As demonstrated by Sun & Sundaresan [90], under dynamic conditions, the stress tracks the average coordination number, $Z$, more closely than the particle volume fraction. Hence it is more accurate to characterize the regimes in terms of $Z$ (and shear rate), than in terms of volume fraction and shear rate. This distinction is more apparent when particles interact cohesively. For non-cohesive assemblies in slow, steady shear, $Z$ falls below $Z_c$, when $\phi$ drops below $\phi_c$. In contrast, for cohesive assemblies, $Z$ can remain large even when $\phi$ is lowered below $\phi_c$, and force chains persist, leading to rate-independent regime. (Compare Figures 2.3(b) and 2.4(b).)

Another behavior connected to the coordination number is the expansion of the cohesive regime with increasing $Bo^*$, as illustrated in Figure 2.3(b). The critical shear rate which sets the boundary between the cohesive and inertial regimes scales with $\sqrt{Bo^*}$, as demonstrated in Figure 2.3(c), where data are collapsed by scaling the dimensionless shear rate with $\sqrt{Bo^*}$. The $\sqrt{Bo^*}$ scaling can readily be rationalized: when cohesive energy ($\sim Bo^*$) is overcome by the kinetic energy supplied by the shearing ($\sim \dot{\gamma}^2$), the system transitions from cohesive regime to inertial regime. This transition in dependence of $Z$ on shear rate between the cohesive regime and inertial regime is consistent with previous findings [57, 79].

Increasing shear rate tends to break down the force chains in the cohesive regime, weakly at low shear rates and rapidly in the vicinity of $\sqrt{Bo^*}$. In contrast, increasing shear rate increases the coordination number in the inertial regime for both cohesive and non-cohesive systems. It is the interplay between these two trends that give rise to a minimum in the magnitude of $Z$ for cohesive systems in the vicinity of $\sqrt{Bo^*}$, and the regime transition observed in the pressure plot (see Figure 2.3(b)).
\hat{\dot{\gamma}} \equiv \dot{\gamma}_d / \sqrt{k/(\rho_s d)}

\begin{align*}
\text{(a) } Z = 0 \\
\text{(b) } Z = 5 \times 10^{-7} \\
\text{(c) } Z = 5 \times 10^{-6} \\
\end{align*}

Figure 2.3: The average coordination number versus scaled shear rate at $\mu = 0.1$ and various modified Bond numbers for (a) $\phi = 0.62$ and (b) $\phi = 0.59$. In (c), the data from (b) are collapsed into one curve by subtracting $Z$ for non-cohesive system from that of cohesive systems and rescaling the shear rate. Hookean contact and van der Waals force model are used here.

\begin{align*}
\text{(a) } \hat{\gamma} \equiv \dot{\gamma}_d / \sqrt{k/(\rho_s d)} \\
\text{(b) } \hat{\gamma} \equiv \dot{\gamma}_d / \sqrt{k/(\rho_s d)} \\
\end{align*}

Figure 2.4: Scaled pressure versus scaled shear rate at $\mu = 0.1$ and various modified Bond numbers for (a) $\phi = 0.62$ and (b) $\phi = 0.59$. Hookean contact and van der Waals force model are used here.
Table 2.1: Values of model constants

<table>
<thead>
<tr>
<th>µ-dependent parameters</th>
<th>µ</th>
<th>(\phi_c)</th>
<th>(\phi_a)</th>
<th>(\epsilon)</th>
<th>(\alpha_{QS})</th>
<th>(\eta_s)</th>
<th>(\alpha_3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>µ</td>
<td>0.1</td>
<td>0.614±0.001</td>
<td>0.45</td>
<td>0.95±0.03</td>
<td>0.36</td>
<td>0.268</td>
<td>0.23</td>
</tr>
<tr>
<td>0.3</td>
<td>0.596±0.001</td>
<td>0.38</td>
<td>0.80±0.03</td>
<td>0.28</td>
<td>0.357</td>
<td>0.23</td>
<td></td>
</tr>
<tr>
<td>0.5</td>
<td>0.587±0.001</td>
<td>0.38</td>
<td>0.67±0.03</td>
<td>0.20</td>
<td>0.382</td>
<td>0.15</td>
<td></td>
</tr>
</tbody>
</table>

| \(\mu\)-independent parameters | \(\alpha_{inert}\) | \(\alpha_{int}\) | \(\alpha_{coh,1}\) | \(\alpha_{coh,2}\) | \(I_0\) | \(\alpha_1\) | \(\beta_1\) | \(\hat{\gamma}_0\) | \(\alpha_2\) | \(\beta_2\) | \(\alpha_4\) |
|-------------------------------|---------|---------|---------|---------|------|-------|--------|------|-------|-------|--------|------|
| 0.021 | 0.099 | 0.15 | 0.008 | 0.32 | 0.37 | 1.5 | 0.1 | 0.2 | 1.0 | 0.1 |

### 2.2.3 Pressure

A blended pressure model has been previously proposed for non-cohesive granular materials, which can capture the pressure continuously across different dense-flow regimes for different volume fractions and shear rates [52]. In this model, \(p_{QS}\), \(p_{inert}\), and \(p_{int}\), which represent pressure in the quasistatic, inertial, and intermediate regimes, are blended to model each regime and the transitions between them. The model is based on the scaling law similar to those in conventional critical phenomena [92, 93]. Specifically, there exists an asymptotic power-law relationship between stress and shear rate for each flow regime \(j\) [52]:

\[
p_j/|\phi-\phi_c| \sim \left[\frac{\dot{\gamma}}{|\phi-\phi_c|}\right]^{m_j},
\]

where \(m_{QS} = 0\), \(m_{inert} = 2\), and \(m_{int} = m^*\). As shown in Figure 2.6, \(p_{inert} \sim |\phi-\phi_c|^{-2}\). Furthermore, the pressure is essentially independent of volume fraction in the intermediate regime [52]. It then follows that \(\omega = (\epsilon + 2)/2\) and \(m^* = 2\epsilon/(\epsilon + 2)\). Accordingly, for non-cohesive particles with Hookean contact,

\[
p = \begin{cases} 
p_{QS} + p_{int} & \text{for } \phi \geq \phi_c \\
\left(p_{inert}^{-1} + p_{int}^{-1}\right)^{-1} & \text{for } \phi < \phi_c,
\end{cases}
\]
where

\[ \frac{p_{QS}d}{k} = \alpha_{QS} |\phi - \phi_c|^\epsilon, \quad (2.7) \]

\[ \frac{p_{\text{int}}d}{k} = \alpha_{\text{int}} \dot{\gamma}^{2\epsilon/(\epsilon+2)}, \quad (2.8) \]

\[ \frac{p_{\text{inert}}d}{k} = \frac{\alpha_{\text{inert}} \dot{\gamma}^2}{|\phi_c - \phi|^2}. \quad (2.9) \]

Here, \( \phi_c = \phi_c(\mu) \), and \( \alpha_{\text{int}} \) and \( \alpha_{\text{inert}} \) are approximately independent of \( \mu \); see Table 2.1. The robustness of Eqn. (2.9) is illustrated in Figure 2.6(a). The scaling exponent \( \epsilon \) and prefactor \( \alpha_{QS} \) in Eqn. (2.7) manifest systematic dependence on \( \mu \), which was not reported by Chialvo et al. [52], who took \( \epsilon = 2/3 \) for all \( \mu \). Although it is not the principal focus of this study, we report in Table 2.1 the best-fit values of \( \epsilon \) and \( \alpha_{QS} \) for three different values. As demonstrated in Figure 2.6(b), Eqn. (2.7) captures the pressure in the quasistatic regime satisfactorily. With the values of \( \epsilon \), the pressure data are collapsed onto two curves (one above \( \phi_c \) and one below) for different particle friction coefficients using the scaling previously discussed, as shown in Figure 2.18.

The pressure model for non-cohesive systems is readily modified to account for the effect of cohesion, as described below. The data reveal two trends which provide clues for constructing simple models. Firstly, as illustrated in Figure 2.7, \( pd/k \sim \text{Bo}^* \) in the cohesive regime for all volume fractions (except for those near \( \phi_c \)). This behavior is consistent with: (a) \( pd/k \sim \dot{\gamma}^2 \) in the inertial regime and (b) the critical \( \dot{\gamma} \) value separating the inertial and cohesive regimes scales as \( \sqrt{\text{Bo}^*} \). Figure 2.7 shows results down only to \( \phi \approx 0.50 \). At lower values of \( \phi \), the flow transitions to shear flows of agglomerates, and the size of the simulation domain used in this study is inadequate to get meaningful results. Secondly, for non-cohesive particles the intermediate asymptote (corresponding to \( \phi = \phi_c \)) takes the form
Figure 2.5: Collapse of pressure versus shear rate curves for (a) \( \mu = 0.1 \), (b) \( \mu = 0.3 \), and (c) \( \mu = 0.5 \). In all cases, the pressure is scaled as \( p^* = p/|\phi - \phi_c|^\epsilon \), and shear rate as \( \dot{\gamma}^* = \dot{\gamma}/|\phi - \phi_c|^{(\epsilon+2)/2} \). (Values for \( \epsilon \) are included in Table 2.1.) Symbols denote simulation results at various volume fractions as per the legend from Figure 1. The functions, described in Eqns. (2.6)–(2.9) and represented by solid lines, captures regime asymptotes as well as transitions. Hookean contact with no cohesion is used.

Figure 2.6: Collapse of pressure for (a) inertial regime and (b) quasi-static regime. For (a), the solid line has a slope of \(-2\) and \(y\)-intercept of 0. For (b), the solid line has a slope of 1 and \(y\)-intercept of 0. All points with different volume fractions and particle friction coefficients fall on the lines. Hookean contact is used.
Figure 2.7: Dimensionless pressure scaled by $Bo^*$ versus volume fraction in the cohesive regime at $\dot{\gamma} = 3.2 \times 10^{-6}$ for $\mu = 0.1$ and various $Bo^*$ values. The line represents $0.15\frac{|\phi - \phi_a|}{|\phi_c - \phi|}$, where $\phi_c(\mu = 0.1) = 0.614$ and $\phi_a(\mu = 0.1) = 0.45$. Hookean contact and van der Waals force model are used here.

\[ p_{\text{int}}d/k = \alpha_{\text{int}}\dot{\gamma}^{2\epsilon/(\epsilon + 2)} \] [52]. While this asymptote persists for cohesive particles at high $\dot{\gamma}$ values, it becomes rate-independent when $\dot{\gamma}$ becomes small compared to $\sqrt{Bo^*}$. Together these observations suggest that, in the vicinity of $\phi_c$, $pd/k$ in cohesive regime scales as $(Bo^*)^{\epsilon/(\epsilon + 2)}$.

Based on these observations, we advance the following simple model:

\[
p = \begin{cases} 
p_{QS} + (p_{\text{int}} + p_{\text{coh},2}) & \text{for } \phi \geq \phi_c \\
\left[\left(\frac{p_{\text{inert}} + p_{\text{coh},1}}{\epsilon} + \left(\frac{p_{\text{int}} + p_{\text{coh},2}}{\epsilon}\right)^{-1}\right)^{-1} & \text{for } \phi < \phi_c,
\end{cases}
\]

(2.10)

where $p_{QS}$, $p_{\text{int}}$, and $p_{\text{inert}}$ are given by Eqns. (2.7)-(2.9), and

\[
p_{\text{coh},1}d/k = \alpha_{\text{coh},1}Bo^*\frac{|\phi - \phi_a|}{|\phi_c - \phi|},
\]

(2.11)

\[
p_{\text{coh},2}d/k = \alpha_{\text{coh},2}(Bo^*)^{\epsilon/(\epsilon + 2)}.
\]

(2.12)
Figure 2.8: Shear stress ratio versus scaled shear rate for (a) non-cohesive particles, (b) cohesive particles with $\text{Bo}^* = 5 \times 10^{-6}$, (c) cohesive particles with $\text{Bo}^* = 5 \times 10^{-5}$. In all cases, Hookean contact and van der Waals force model are used, and interparticle friction coefficient $\mu = 0.1$. Symbols denote simulation results at various volume fractions as per the legend from Figure 2.2. Lines denote model predictions from Eqns. (2.13) - (2.15) and (2.18).

For non-cohesive particles, where $\text{Bo}^* = 0$, $p_{\text{coh},1}$ and $p_{\text{coh},2}$ vanish, and the proposed model returns to its original form written for non-cohesive particles. The model constants are provided in Table 2.1. Only $\epsilon$, $\alpha_{\text{QS}}$, $\phi_c$, and $\phi_a$ need to be adjusted as functions of $\mu$ (see Table 2.1). Predictions based on this pressure model are compared with the simulation results in Figure 2.2. The proposed model captures the data reasonably well not only in each regime but also in the transition regions.

### 2.2.4 Shear stress ratio

Figure 2.8 displays the variation of stress ratio $\eta$ ($= \tau/p$) with the scaled shear rate $\dot{\gamma}$ for both non-cohesive and cohesive particles with $\mu = 0.1$. Cohesion has a significant effect on the stress ratio only in the cohesive regime, where cohesion increases the stress ratio appreciably. This increase in stress ratio due to cohesion is in agreement with prior experiments [81] and simulations [57, 58, 82]. It is also consistent with increasing average coordination number with the inclusion of cohesion in the cohesive regime.
The stress ratio model for non-cohesive frictional granular materials proposed by Chialvo et al. [52] is composed of two contributions, $\eta_{\text{hard}}$ and $\eta_{\text{soft}}$. The term $\eta_{\text{hard}}$ is a function of inertial number $I \equiv \dot{\gamma} d / \sqrt{p/\rho_s}$ and describes the shear stress ratio for infinitely hard particles, while $\eta_{\text{soft}}$ is a function of $\dot{\gamma}$ and describes the deviation from hard-particle behavior due to finite stiffness:

$$
\eta^* = \eta_{\text{hard}}(I) - \eta_{\text{soft}}(\dot{\gamma}),
$$

(2.13)

$$
\eta_{\text{hard}}(I) = \eta_s(\mu) + \frac{\alpha_1}{(I_0/I)^{\beta_1} + 1},
$$

(2.14)

$$
\eta_{\text{soft}}(\dot{\gamma}) = \eta_s(\mu) + \frac{\alpha_2}{(\dot{\gamma}_0/\dot{\gamma})^{\beta_2} + 1}.
$$

(2.15)

Here, $\eta^*$ is the stress ratio for non-cohesive granular materials, and $\eta_s$ is the yield stress ratio.

As shown below, the well-known Mohr-Coulomb relation $\tau = \eta^* p + C$, which can be cast as $\eta = \eta^* + C/p$, captures our steady, simple shear flow simulation results in the rate-independent regimes, namely quasistatic and cohesive regimes, provided $C$ is properly modeled. Rognon et al. [58] found that the model proposed by Rumpf [94] for $C$, $C_{\text{Rumpf}} = Z \eta^* \phi Bo^* k/ (\pi d)$, overestimates the value of $C$ needed to match the simulation results. We found the same to be true as well. It is now known that Rumpf’s formula does not account for non-affine particle displacements [95–98], which arise due to the structural disorder in the system. Upon correcting for non-affine displacement [95–98],

$$
C_{\text{Rumpf}}^{\text{corr}} = (Z - Z_n) \eta^* \phi Bo^* k/ (\pi d)
$$

(2.16)
As shown in Figure 2.9, our simulation results are captured nicely if $Z_n$ is set to be 3. This choice of $Z_n$ differs from $Z_n = 2.4$ determined by Zaccone [98], which may be attributed to different models for interaction between particles used in our and Zaccone’s studies.

In the quasistatic and cohesive regimes, $\eta^*$ is essentially $\eta_s$, and $Z$ does not vary significantly with the shear rate (e.g., see Figures 2.3(a)(b)) and volume fraction (see results for the case of Hookean contact and van der Waals force model shown in Figure 2.10). In views of these, and since the coordination number is not directly accessible, a lumped model constant $\alpha_3 = (Z - Z_n) \eta_s / \pi$ is used. The stress ratio model for cohesive granular materials in the quasistatic and cohesive regime then becomes,

$$\eta = \eta^* + \frac{\alpha_3 \phi Bo^* k/d}{p}.$$  \hfill (2.17)
To extend this model to cover rate-dependent regimes, namely inertial and intermediate, we modify the model as:

\[
\eta = \eta^* + \frac{\alpha_3 \phi Bo^* k/d}{p} \frac{1}{\frac{\dot{\gamma}}{\alpha_4 \sqrt{Bo^*}} + 1}.
\]  

(2.18)

Here, \( \alpha_4 \sqrt{Bo^*} \) approximates the critical shear rate which separates the cohesive and inertial regimes. When \( \dot{\gamma} \ll \alpha_4 \sqrt{Bo^*} \), the model returns to Eqn. (2.17). When \( \dot{\gamma} \gg \alpha_4 \sqrt{Bo^*} \), the second term in the model vanishes. The model describes stress ratio reasonably well for all \( Bo^* \) values considered without any changes to constitutive parameters, and for different \( \mu \) values with slight adjustment of \( \alpha_3 \). The values for \( \alpha_3 \) and \( \alpha_4 \) are listed in Table 2.1.

![Figure 2.10: The average coordination number versus volume fraction in the cohesive regime for particles with \( \mu = 0.1 \) and \( Bo^* = 5 \times 10^{-5} \).](image)

**2.2.5 Generality of the results**

The newly identified regime map is preserved when the Hookean contact model is replaced by a Hertzian contact model as well as when the van der Waals force model is replaced with the alternate cohesion model of Rognon et al. [58]. The general form of the stress model is also preserved, albeit with small modifications. We illustrate these points by presenting two
Figure 2.11: Scaled pressure versus scaled shear rate for (a) Hertzian contact and the van der Waals force model, (b) Hookean contact and the alternative cohesion model [58]. Here, $\mu = 0.1$ and $Bo^* = 5 \times 10^{-5}$. Symbols denote simulation results at various volume fractions as per the legend from Figure 2.2. Lines denote model predictions from Eqns. (2.10) and (17) - (21) in (a), and Eqns. (2.10) - (2.12) in (b).

Flow regimes

Figures 2.11(a) and (b) show the variation of scaled pressure against the scaled shear rate for cohesive particles from these two particle-scale models. The cohesive regime, characterized by rate-independent behavior below the critical volume fraction ($\phi_c = 0.614$ for $\mu = 0.1$ in the figures) and lower shear rates, is clearly present in both cases. In addition, simulation results from different $Bo^*$ values confirm that the critical shear rate, separating the cohesive and inertial regimes, scales with $\sqrt{Bo^*}$ for both cases (not shown).
Pressure

For case (a), as in non-cohesive systems [52], \( p_{\text{inert}} \sim |\phi_c - \phi|^{5/3} \). As a result, \( \omega = (\epsilon + 5/3)/2 \) and \( m^* = 2\epsilon/(\epsilon + 5/3) \). Hertzian contact requires the following modifications to the contributions \( p_{QS}, p_{\text{inert}}, \) and \( p_{\text{int}} \) to Eqn. (2.10):

\[
p_{QS}/k = \alpha_{QS}|\phi - \phi_c|^{\epsilon},
\]

\[
p_{\text{int}}/k = \alpha_{\text{int}} \dot{\gamma}^{2\epsilon/(\epsilon + 5/3)},
\]

\[
p_{\text{inert}}/k = \frac{\alpha_{\text{inert}} \dot{\gamma}^2}{|\phi_c - \phi|^{5/3}}.
\]

It is noted that Eqn. (2.19) is the same as the Eqn. (2.7) except for scaling on the left-hand side. However, the values of \( \epsilon \) are different from the ones for Hookean contact. It is found
that $\epsilon = 1.35, 1.20, \text{and} 1.10$ with uncertainties of $\pm 0.03$ for $\mu = 0.1, 0.3, \text{and} 0.5$, respectively. The value of $\epsilon$ for Hertzian contact is approximately $3/2$ times the one for Hookean contact, which is consistent with previous results [90, 99]. Using the values for $\epsilon$, the pressure data can now be collapsed onto two curves for different $\mu$, as illustrated in Figure 2.13 for the case of $\mu = 0.1$. Thus, Hertzian and Hookean contacts afford similar simulation results such that pressure can be collapsed in a similar fashion.

The first cohesive contribution $p_{\text{coh},1}$ remains unchanged from Eqn. (2.11) except for scaling on the left-hand side:

$$p_{\text{coh},1}/k = \alpha_{\text{coh},1} B_0^* \frac{|\phi - \phi_c|}{|\phi_c - \phi|}. \quad (2.22)$$

Finally, since $p_{\text{coh},2}$ modifies the intermediate-regime contribution ($p_{\text{int}}/k \sim \dot{\gamma}^{2/[(\epsilon+5)/3]}$) and their sum becomes rate-independent for $\dot{\gamma} \ll \sqrt{B_0^*}$, it is modified to scale as $B_0^* \dot{\gamma}^{2/[(\epsilon+5)/3]}$. 

Figure 2.13: Collapse of pressure versus shear rate curves for $\mu = 0.1$. The pressure is scaled as $p^* = p/[\phi - \phi_c]^{\epsilon}$, and shear rate as $\dot{\gamma}^* = \dot{\gamma}/[\phi - \phi_c]^{(\epsilon+5)/3}/2$. $\epsilon = 1.35$ is used. Symbols denote simulation results at various volume fractions as per the legend from Figure 1. The blending function, described in Eqns. (2.19)–(2.21) and represented by solid lines, captures regime asymptotes as well as transitions. Hertzian contact with no cohesion is used.
This term now becomes

\[ p_{\text{coh},2}/k = \alpha_{\text{coh},2}(B_o^*)^{(\epsilon + 5/3)}. \]  

(2.23)

Model parameters used in the lines shown in Figure 2.11(a) are: \( \epsilon = 1.35, \alpha_{\text{QS}} = 0.11, \alpha_{\text{int}} = 0.05, \alpha_{\text{inert}} = 0.13, \alpha_{\text{coh},2} = 0.006. \) Values for \( \phi_c, \phi_a, \) and \( p_{\text{coh},1} \) are the same as those for Hookean contact with van der Waals force model (see Table 2.1).

For case (b), the functional forms for the pressure model are unchanged, and Eqns. (2.7) – (2.12) are applied. Only values for \( \phi_a, \alpha_{\text{coh},1}, \) and \( \alpha_{\text{coh},2} \) are now different: \( \phi_a = 0.50, \alpha_{\text{coh},1} = 1.2, \alpha_{\text{coh},2} = 0.025. \)

Shear stress ratio

Stress ratio models are slightly modified for both cases and compared with the simulation data in Figures 2.12(a) and (b). For case (a), \( Z_n = 3 \) captures our simulation results, and since \( Z \) does not change significantly with volume fraction (see results for the case of Hertzian contact and van der Waals force model shown in Figure 2.10), we can continue to lump \( (Z - Z_n) \eta_s/\pi \) as \( \alpha_3. \) As a result of change in the dimension of \( k \) for the Hertzian contact, Eqn. (2.18) now reads:

\[ \eta = \eta^* + \frac{\alpha_3 \phi B_o^* k}{\sqrt[4]{\eta^*} + 1}, \]  

(2.24)

where \( \eta^* \) is described in Eqns. (2.13) – (2.15). Model parameters used in the lines shown in Figure 2.12(a) are: \( \alpha_1 = 0.27, \alpha_2 = 0.23, \beta_1 = 1.0, \alpha_4 = 3. \) Values for all the other parameters are the same as those for Hookean contact with the van der Waals force model.

For case (b), \( Z_n = 0.5 \) captures our simulation results adequately. Since \( Z \) changes significantly with volume fraction (see results for the case of Hookean contact and the alternative
cohesion model shown in Figure 2.10), we find that modeling \((Z - Z_n)\eta_s/\pi\) as \(\alpha_5(\phi - \phi_a)\) with \(\alpha_5 = 10.3\) captures the stress ratio data well. As a result, Eqn. (2.18) is modified to the following:

\[
\eta = \eta^* + \frac{\alpha_5(\phi - \phi_a)Bo^*k/d}{p} \frac{1}{\frac{1}{\alpha_4^2Bo^*} + 1},
\]

where \(\alpha_4 = 0.5\). The solid lines in Figure 2.12(b) correspond to Eqn. (2.25). Good agreement with simulation results is readily seen.

Note that different expressions for \((Z - Z_n)\eta_s/\pi\) are needed to capture stress ratio results for van der Waals force model and alternative cohesion model. As noted earlier, the two cohesion models are significantly different: the van der Waals force saturates when the particles come to contact, while the cohesion is only present when the particles are in contact in the alternative cohesion model. Figure 2.10 illustrates the dependence of the coordination number on volume fraction for the three different cases presented in this article. For Hookean contact and van der Waals force model, \(Z\) is roughly independent from \(\phi\); for Hertzian contact and van der Waals force model, \(Z\) shows slight dependence on \(\phi\); and for Hookean contact and alternative cohesion model, \(Z\) increases appreciably with \(\phi\). This difference in response of coordination number to volume fraction helps explain the necessity of different expressions for \((Z - Z_n)\eta_s/\pi\).

\[\text{2.2.6 Conclusions}\]

We have investigated shear flows of dense cohesive granular materials via DEM simulations. The quasistatic and intermediate regimes observed for non-cohesive particles persist for cohesive particles, while the inertial regime of non-cohesive particles bifurcates into two regimes: rate-independent cohesive regime at low shear rates and inertial regime at higher shear rates. The regime map for the rheology of dense assemblies of cohesive particles is
found to be robust even when the particle-scale details of the model are altered. Furthermore, the pressure and shear stress ratio results obtained in our simulations can be captured via simple algebraic expressions that can be used in conjunction with continuum models for flows in practical devices.

2.3 Rheology of granular materials with particle size distributions.

2.3.1 Introduction

Real particles often have particle size distributions (PSD). To take account of polydispersity, new kinetic theory has been developed for granular flow (e.g. [100–104]). However, it is limited to dilute systems and does not account for friction. Although a few studies have appeared in the literature on dense-flow rheology with polydispersity, they are limited to binary mixtures [17, 60, 105, 106], or mixtures with four particle sizes [67]. It is not known at this time whether a single rheological model that can describe dense flows of granular mixtures of any size distribution with fair accuracy. The present study demonstrates that it is indeed possible.

In this present study, we investigate the rheology of granular materials with various size distributions through DEM simulations of simple shear flows of frictional particles. Most of the simulations are performed using Hertzian contact model. To test the robustness, a few simulations with Hookean contact model have also been performed. We perform simulations for four types of PSDs (binary, linear, Gaussian, and lognormal), and demonstrate that the different regimes observed for monodisperse particles persist even when size distribution is included. The jamming volume fraction that separates the quasistatic and inertial regimes is found to increase when particles manifest size distribution. We further demonstrate that
pressure can be scaled by powers of the distance to the jamming volume fraction, in the same manner as was done for the case of uniformly sized particles [52], provided that we recognize that the jamming volume fraction and the effective particle size change with PSD. We then show that these jamming volume fractions used for collapse of pressure can be expressed as a function of polydispersity and skewness of the PSD. Finally, for shear stress ratio (ratio between shear stress and pressure), we demonstrate that the inertial number model is still valid for particles with size distributions, provided that the yield stress ratio is adjusted to account for PSD. Thus, we are able to extend the stress model proposed by Chialvo et al. [52] for dense flows of frictional particles with same size to account for frictional particles with any size distribution.

2.3.2 Particle size distributions

Following the study on jamming behaviors in a static system [107], four types of distributions \( P(r) \) of radii \( r \) are studied: binary, linear, Gaussian, and lognormal. \( P(r) \) is a number-based continuous distribution, and is normalized to unity, \( \int P(r)dr = 1 \). The distributions are illustrated in Figure 2.14. We also include a monodisperse case as the base case.

For monodisperse case, all particles have the same scaled radius of 0.5. The binary distribution consists of particles with two distinct radii, \( r_1 \) and \( r_2 \), where \( r_1 = 0.5 \) and \( 0.05 \leq r_2 \leq 0.5 \). The distribution is of the form \( P(r) = (1 - f_r)\delta(r - r_1) + f_r\delta(r - r_2) \), where \( f_r \) is the number fraction for particles with radii of \( r_2 \), and \( \delta(x) \) is the Dirac delta function. The linear distribution is of the form \( P(r) = Ar + B \), where the distribution in particle size exists over a finite range between \( a \) and \( b \), with \( 0.05 \leq a < b \leq 0.5 \). The Gaussian distribution is of the form \( P(r) = A_G\exp\left[-(r - \lambda)^2/(2\sigma^2)\right] \), where \( \lambda \) is the mean and set to 0.25, \( \sigma \) is the standard deviation, and \( A_G = 1/(\sqrt{2\pi}\sigma^2) \). The lognormal distribution is of the form \( P(r) = A_L\exp\left\{-\ln(r - m)^2/(2s)^2\right\} \), where \( A_L = 1/(r\sqrt{2\pi}s^2) \). \( m \) and \( s \) are log mean and log
Figure 2.14: Illustrations of various PSD considered in the study as per the legend. For binary distribution, $f_r = 0.3$, $r_1 = 0.5$, and $r_2 = 0.25$. For linear distribution, $A = 5$, $B = 1$, $a = 0.1$, and $b = 0.5$. For Gaussian distribution, $\lambda = 0.25$, and $\sigma = 0.05$. For lognormal distribution, $\lambda = 0.2$, and $\sigma = 0.003$.

standard deviation respectively, and are associated with $\lambda$ and $\sigma$ as, $m = \ln(\lambda^2/\sqrt{\sigma + \lambda^2})$ and $s = \sqrt{\ln(\sigma/\lambda^2 + 1)}$. $\lambda$ is set to 0.2.

Each size distribution can be characterized by polydispersity

$$\delta = \frac{\sqrt{\langle \Delta r^2 \rangle}}{\langle r \rangle}, \quad (2.26)$$

and skewness

$$S = \frac{\langle \Delta r^3 \rangle}{(\langle \Delta r^2 \rangle)^{3/2}}. \quad (2.27)$$

Polydispersity $\delta$ and skewness $S$ measure the spread and shape of the distribution respectively. In the equations, $\Delta r = r - \langle r \rangle$, and the moments of $r$ and $\Delta r$ are defined as $\langle r^n \rangle = \int r^n P(r) \, dr$ and $\langle \Delta r^n \rangle = \int \Delta r^n P(r) \, dr$, respectively. Consistent with the previous study [107], $\delta$ equal to 0.1, 0.15, 0.25, and 0.4 are considered. For the binary distributions, $r_2$ and $f_r$ are adjusted to yield several values of $S$ for each $\delta$ value. Similarly, for the linear
distributions, $A$, $B$, $a$, and $b$ are chosen (with the constraint of $\int_a^b P(r)dr = 1$) to yield several values of $S$ for each $\delta$ value. For both Gaussian and lognormal distributions, $\sigma$ is adjusted to yield each $\delta$ value. As a result, $S$ is prespecified in the Gaussian and lognormal distributions. For the continuous size distributions (linear, Gaussian, and lognormal), random numbers are generated for $r$ to yield the desired size distribution $P(r)$. For each size distribution, scaled radii are limited between 0.05 and 0.5. For continuous size distributions, at large polydispersity values, a tiny fraction of particles generated have radii slightly outside the range. For those particles, the radii are set to 0.05 in the case of $r < 0.05$ or 0.5 in the case of $r > 0.5$. Thus, the distributions are only slightly altered in these cases.

As shown in Eqns. (2.1) and (2.2), for Hertzian contact model, $f$ term is included that accounts for relative particle sizes. Thus, as Hertizan contact better accounts for polydispersity, it is the primary focus of the study and used to simulate the systems for all the size distributions. To demonstrate the robustness of the results, simulations are repeated using Hookean contact for both the binary and lognormal size distributions with $\delta$ of 0.25 and 0.4.

### 2.3.3 Flow regimes

In most of the simulations reported here, particle friction coefficient $\mu = 0.5$ is used, representing a typical value for granular materials. As discussed later, the conclusions drawn in the study here are applicable for other $\mu$ values as well, only requiring slight modifications to certain model parameters as detailed previously for monodisperse particles [52] as well as in Table 2.1. For each size distribution, simulations are performed for various shear rates and volume fractions.

Figure 2.15(a) plots the scaled pressure $p/k$ against the scaled shear rate $\dot{\gamma} = \gamma d/\sqrt{k/\rho_s}$ for monodisperse particles using Hertzian contact. Three regimes are present [52, 63–65]: quasistatic at low shear rates and high volume fractions, inertial at low shear rates and
low volume fractions, and intermediate at high shear rates and all volume fractions. The quasistatic and inertial regimes are separated by a critical volume fraction $\phi_c$ which is a function of $\mu$ as found previously [52]. When the assembly becomes polydisperse, it is found that this regime map is preserved while the value of $\phi_c$ changes slightly. To illustrate, the case of lognormal distribution with $\delta = 0.25$ is shown in Figure 2.15(b). The three regimes are observed. However, the volume fraction of 0.59, residing in the quasistatic regime at lower shear rates for monodisperse particles, is now in the inertial regime, indicating an increased value of $\phi_c$.

For monodisperse particles, it has been shown that stresses fluctuate in large magnitude near $\phi_c$ as force chains are constantly broken and formed during the shearing process. The same fluctuation is observed for polydisperse particles as well, as seen in Figure 2.16(a) for the particles of lognormal distribution with $\delta = 0.25$. To characterize the magnitude of the fluctuations, the standard deviation of pressure $\sigma_p = \sqrt{\langle p^2(t) \rangle - \langle p(t) \rangle^2}$ is scaled by the time-average pressure $p$ at various $\phi$ [52]. As seen in Figure 2.16(b), there exists a spike at $\phi_{c,PSD} = 0.605$ for the particles of lognormal distribution with $\delta = 0.25$. For comparison, the
Figure 2.16: Transition of pressure fluctuations between inertial and quasistatic regimes. (a) Pressure fluctuations in time are observed to become larger near the critical point. Particles of lognormal distribution with $\delta = 0.25$ are used. (b) The standard deviation of pressure, scaled by the mean pressure, exhibits a spike at $\phi_c$ for both monodisperse and polydisperse particles. The critical volume fraction for polydisperse particles $\phi_c^{PSD}$ is larger than the one for monodisperse particles $\phi_c^{mono}$. Polydisperse particles are of lognormal distribution with $\delta = 0.25$. In all cases, Hertzian contact is used with $\mu = 0.5$.

case of monodisperse particles is included in the figure as well, where a spike is observed at $\phi_c^{mono} = 0.587$. Thus, the figure further illustrates that $\phi_c$ increases when particles become polydisperse.

As expected, different values of $\phi_c$ would be obtained for different size distributions $P(r)$. The dependence of $\phi_c$ on $P(r)$ is explored and discussed in detail in the next section.

### 2.3.4 Pressure

As discussed already in the first part of this chapter, it has been shown in experimental [68] and computational [52, 64, 66, 67, 108] studies of monodisperse particles that pressure vs. shear rate data at several different volume fractions will collapse onto two curves (one above $\phi_c$ and one below) upon scaling the pressure and shear rate by powers of $|\phi - \phi_c|$, the distance to jamming. As seen in Figure 2.17(a), pressure vs. shear rate data for monodisperse particles
from Figure 2.15(a) collapse onto two curves with $p^* = (p/k)/|\dot{\phi} - \phi_c|^\epsilon$ and $\dot{\gamma}^* = \dot{\gamma}/|\dot{\phi} - \phi_c|^{(\epsilon + \chi)/2}$.

As determined in the first part of this chapter, $\epsilon = 1.1$ and $\chi = 1.43$ are used. As shown in Figure 2.17(a), the two curves from collapse are captured by models represented as solid lines, which are developed in the first part of this chapter. The details and derivations of the models would be presented later in this section. For convenience of the discussions in the next few paragraphs, we include the models describing the collapse of pressure here:

$$p^* = \begin{cases} 
0.06 + 0.075\dot{\gamma}^*^{0.87} & \text{for } \phi \geq \phi_c \\
(0.17\dot{\gamma}^*-2 + 0.075\dot{\gamma}^*-0.87)^{-1} & \text{for } \phi < \phi_c.
\end{cases}$$ (2.28)

The two cases ($\phi \geq \phi_c$ and $\phi < \phi_c$) in the equations above represent the two curves in the collapse.

It is found that the same collapse can be achieved for polydisperse particles with the same $\epsilon$ and $\chi$ values. As shown in Figure 2.17(b), pressure vs. shear rate data for particles of the lognormal distribution from Figure 2.15(b) also collapse onto two curves with the same scaling. $\phi_c = 0.605$, obtained in the previous section, is used for the scaling. Same collapses using different $\phi_c$ values are obtained for other size distributions as well.

If quantities are scaled properly, the two curves from collapse obtained from all size distributions should all overlap with the ones from the monodisperse case. As noted before, we consider three options of effective diameter $\bar{d}$ for such scaling: volume-averaged diameter $d_{43}$, Sauter-mean diameter $d_{32}$, and root-mean-cubed diameter $d_{rmc}$. The options are compared based on evaluating the difference between collapses from various size distributions and the collapse from monodisperse case which can be represented by Eqn. (2.28). Specifically, in a given collapse from a PSD, for each data point ($\dot{\gamma}^* = \dot{\gamma}^*_{data}$ and $p^* = p^*_{data}$), we compare the percent difference ($\Delta_{p^*}$) between $p^*_{data}$ and the value predicted from Eqn. 2.28 ($p^*_{predict}$) using $\dot{\gamma}^* = \dot{\gamma}^*_{data}$. Percent difference $\Delta_{p^*}$ can thus be calculated as $|p^*_{predict} - p^*_{data}|/p^*_{data}$. For each option of $\bar{d}$, $\Delta_{p^*}$ is computed for each data point for various distributions (including lin-
Figure 2.17: Collapse of pressure versus shear rate curves for (a) monodisperse particles, (b) particles of lognormal distribution with \( \delta = 0.25 \), and (c-d) particles of all size distributions considered in this study (binary, linear, Gaussian, and lognormal distributions as well as monodisperse particles). In all cases, the pressure is scaled as \( p/|\phi - \phi_c\|^{\epsilon} \), and shear rate as \( \dot{\gamma}/|\phi - \phi_c|^{(\epsilon+\chi)/2} \). For scaling, \( d_{43} \) is used in (b) and (c), and \( d_{32} \) is used in (d). In (a), \( \phi_c = 0.587 \) is used. In (b), \( \phi_c = 0.605 \) is used. In (c) and (d), \( \phi_c \) values reported in Figure 2.19 are used. Symbols denote simulation results at various volume fractions as per the legend from Figure 2.15. The function of Eqn. (2.28) represented by solid lines captures regime asymptotes as well as transitions. In all cases, Hertzian contact is used with \( \mu = 0.5 \).
Figure 2.18: Collapse of pressure versus shear rate curves for particles of (c) particles of various size distributions (binary and lognormal distributions with $\delta = 0.4$ as well as monodisperse particles). In all cases, the pressure is scaled as $p/|\phi - \phi_c|$, and shear rate as $\dot{\gamma}/|\phi - \phi_c|^{(\epsilon+\chi)/2}$. $\phi_c$ values reported in Figure 2.19 are used. Symbols denote simulation results at various volume fractions as per the legend from Figure 2.15. The blending function, described in Eqns. (2.30) – (2.33) (replacing $p_j/k$ with $p_jd_{43}/k$) and represented by solid lines, captures regime asymptotes as well as transitions. The model parameters are the same as those in Figure 2.15. $\chi = 2.14$, $\epsilon = 0.67$, $\alpha_{QS} = 0.2$, $\alpha_{int} = 0.1$, and $\alpha_{inert} = 0.015$. Hookean contact is used with $\mu = 0.5$.

Thus, volume-averaged diameter $d_{43}$ is found a more suitable particle diameter than Sauter-mean diameter $d_{32}$ and root-mean-cubed diameter $d_{rmc}$, confirming previous studies on dense granular rheology of binary mixtures [17, 60]. But it should indeed be noted that the difference between the different choices for diameters is not very large, and hence one can use any of them with nearly comparable levels of accuracy. As noted before, the radii considered in this study are confined between 0.05 and 0.5. As a result, $d_{43}$, $d_{32}$, and $d_{rmc}$ are close to each other. To differentiate them would require a larger range of particle sizes. As shown in Figures 2.17(c) and (d), using volume-averaged diameter $d_{43}$ or Sauter-mean diameter $d_{32}$ for scaling, the resultant two curves from the collapses for all the size distributions considered...
in this study (including monodisperse) overlap equally well. In what follows, we have simply applied \(d_{43}\).

Similar to Hertzian contact as shown in Figures 2.17(c) and (d), same overlap can be achieved for Hookean contact as well, as shown in Figure 2.18. It is noted that essentially the same values of \(\phi_c\) are obtained for Hertzian and Hookean contacts for a given size distribution. These results suggest that the pressure model previously proposed by Chialvo et al. [52] for monodisperse particles is valid for polydisperse particles as well, requiring only two changes. \(d\) is now replaced with a mean diameter, which we have chosen in what follows to be \(d_{43}\). \(\phi_c\) which is only a function of \(\mu\) for monodisperse particles now also depends on size distributions.

We then examine how the value of \(\phi_c\) can be correlated to size distribution \(P(r)\). It has already been found [107] that the jamming volume fraction for a static, frictionless system can be described by \(\delta\) and \(S\) alone with fair accuracy. As shown in Figure 2.19, same conclusion is applicable for the current system. In the figure, \(\phi_c\) is plotted against skewness \(S\) with colors denoting different polydispersity values \(\delta\). The symbol types indicate the corresponding types of size distribution. The figure indicates that regardless of the types of size distribution, \(\phi_c\) can be expressed to a good accuracy in terms of \(S\) and \(\delta\) alone.

The dependence of the critical volume fraction on \(\delta\) and \(S\) is also similar to the one previously observed for static, frictionless particles [107]. Specifically, for a given polydispersity \(\delta\), \(\phi_c\) increases linearly with increasing \(S\). For negative skewness (there are more bigger particles than smaller particles), the polydispersity \(\delta\) has weaker impact on \(\phi_c\) compared with the case of positive skewness (there are more smaller particles than bigger particles). As explained previously [107], for negative skewness, as the particle volume scales with \(r^3\), larger particles occupy much larger volume than smaller particles. Thus, the system is essentially composed of big particles packing like low-polydispersity sample and small particles occupying a negligible portion. For positive skewness, increasing polydispersity \(\delta\) results in greater number of
small particles. $\phi_c$ is thus increased as small particles are able to find spaces between larger particles. As proposed for jamming volume fraction in a static, frictionless system [107], $\phi_c$ can be related to $\delta$ and $S$ by the following empirical relation,

$$\phi_c = \phi_{c\text{mono}}(\mu) + c_1(\mu)\delta + c_2(\mu)S\delta^2.$$  (2.29)

For $\mu = 0.5$ here, $\phi_{c\text{mono}} = 0.587$, $c_1 = 0.0496$, and $c_2 = 0.1039$. For monodisperse particles ($\delta = 0$ and $S = 0$), $\phi_c$ is reduced to $\phi_{c\text{mono}}$, which depends on particle friction coefficient $\mu$ as determined previously [52, 90]: $\phi_{c\text{mono}} = 0.058e^{-5\mu} + 0.582$. As denoted by the lines in Figure 2.19, Equation (2.29) describes $\phi_c$ reasonably well. We also investigated whether jamming volume fraction $\phi_c$ could be correlated in terms of volume-based statistics, but found that it was much easier to correlate the results in terms of number-based statistics as shown above. As $\phi_c$ cannot be larger than unity for any system, this equation could fail for systems with extremely large polydispersity. So one needs to make sure that $\phi_c$ predicted by Eqn. (2.29) is reasonable. In many industrial applications, size ratio of 3 : 1 between large and small particles is quite typical; a binary mixture with 10 vol% of the smaller particles is predicted to have a $\phi_c$ of 0.6557 when the particle friction coefficient is $\mu = 0.5$, which is only marginally higher than the monodisperse case and the equation is applicable.

As mentioned before, the new pressure model for particles with several different size distributions requires only two changes to the model for monodisperse particles. Here, we repeat the same analysis performed for monodisperse particles [52] with those two changes in mind. Specifically, the collapse in Figures 2.17 and 2.18 suggest that there exists a power-law relationship between pressure and shear rate in each flow regime [52]:

$$\frac{p_j}{[\phi - \phi_c]} \sim \left[ \frac{\dot{\gamma}}{[\phi - \phi_c]} \right]^{m_j},$$

$j = \text{QS, int, inert}$. Here, QS, int, and inert indicate properties belonging to quasistatic, intermediate, and inertial regimes respectively. In the rate-independent quasistatic regime, $m_{\text{QS}} = 0$. In the inertial regime, since pressure varies as the square of shear rate, $m_{\text{inert}} = 2$. Thus, assuming $p_{\text{inert}} \sim |\phi - \phi_c|^{-\chi}$, we set $\omega = (\epsilon + \chi)/2$. In addition, as the pressure becomes
Figure 2.19: The dependence of jamming volume fractions $\phi_c$ on polydispersity $\delta$, skewness $S$, and types of size distribution. The values of $\phi_c$ are used to collapse pressure as shown in Figures 2.17 and 2.18. The colors indicate different $\delta$ values. The symbol types correspond to different types of size distribution. The lines denote the model predictions using Eqn. (2.29), where $\phi_c^{\text{mono}} = 0.587$, $c_1 = 0.0496$, and $c_2 = 0.1039$.

effectively independent of $|\phi - \phi_c|$ in the vicinity of the intermediate asymptote, we deduce that $m_{\text{int}} = \epsilon/\omega = 2\epsilon/(\epsilon + \chi)$. Thus, for particles of any size distribution with Hertzian contact,

$$p_{\text{QS}}/k = \alpha_{\text{QS}}|\phi - \phi_c|^{\epsilon},$$

(2.30)

$$p_{\text{int}}/k = \alpha_{\text{int}}\hat{\gamma}^{2\epsilon/(\epsilon + \chi)},$$

(2.31)

$$p_{\text{inert}}/k = \frac{\alpha_{\text{inert}}\hat{\gamma}^{2}}{|\phi_c - \phi|^\chi}. $$

(2.32)

$\hat{\gamma}$ is now $\gamma d_{43}/\sqrt{k/\rho_s}$, and $\phi_c$ is described using Eqn. (2.29). For Hookean contact, $p_j/k$ is replaced by $p_j d_{43}/k$, and $\hat{\gamma} = \gamma d_{43}/\sqrt{k/(\rho_s d_{43})}$. Model parameters ($\alpha_{\text{QS}}, \alpha_{\text{int}}, \alpha_{\text{inert}}, \epsilon,$ and $\chi$) have been determined previously [52].

To describe the transitions between the regime limits which are now modeled by Eqns. (2.30)-(2.32), a blending function $B$ of the form $B(y_1, y_2) = (y_1^w + y_2^w)^{1/w}$ is used. $w = 1$ is used to yield an additive blend for the quasistatic-to-intermediate transition, and $w = -1$ is used to create a harmonic blend for the inertial-to-intermedaite transition. Thus, the pressure
model for particles of any size distribution is the following:

\[
p = \begin{cases} 
  p_{QS} + p_{\text{int}} & \text{for } \phi \geq \phi_c \\
  \left( p_{\text{inert}}^{-1} + p_{\text{int}}^{-1} \right)^{-1} & \text{for } \phi < \phi_c.
\end{cases}
\]

(2.33)

As shown in Figures 2.15, 2.17, and 2.18, this blended pressure model is able to capture the pressure continuously at the regime limits and the transitions.

If we combine Eqns. (2.30)-(2.32) and (2.33), and substitute using the definitions of \( p^* \) and \( \dot{\gamma}^* \), we can arrive at Eqn. (2.28), which describes the two curves from the collapse of pressure as shown using solid lines in Figures 2.17(a-d).

It has been noted previously [90] that the the average contact coordination number \( Z_2 \) tracks pressure in the quasistatic regime more closely than particle volume fraction (as in Eqn. (2.30)) under both steady and dynamic flow conditions. Here, average coordination number is defined as \( Z_2 = 2n_c/n \), where \( n_c \) is the total number of contacts and \( n \) is the total number of particles in the system. Since stress in the quasistatic regime is principally transmitted through force chains, in computing \( Z_2 \), particles with 0 (floaters) or 1 contact (rattlers) are excluded as they are not involved in the force chains (e.g., see [90, 109]). For monodisperse particles, it is found that the scaled pressure in the quasistatic regime (\( p_{QS}/k \) for Hertzian contact and \( p_{QS}d_{43}/k \) for Hookean contact) can be expressed as \( \alpha_{Z_2}(Z_2 - Z_{2c})^\omega \) [90], with \( \omega = 3 \) for Hertzian contact and \( \omega = 2 \) for Hookean contact. \( Z_{2c} \) is a microstructural analog of \( \phi_c \), above which quasistaic regime occurs [90, 91]. The values of \( Z_{2c} \) for monodisperse particles depend on particle friction coefficient \( \mu \) and are found before [90]. \( Z_{2c} = 4.26 \) for \( \mu = 0.5 \) [90]. As shown in Figures 2.20(a) and (b), the relation applies for polydisperse particles as well, with no changes in \( Z_{2c} \) and \( \omega \). It should be noted that, unlike the relationship using \( \phi \) (as in Eqn. (2.30) ), the exponent \( \omega \) is independent of \( \mu \). Furthermore, as \( \phi_c \) changes with different size distributions, \( Z_{2c} \) remains constant. However, unlike \( \phi_c \) whose value can be roughly described with \( \delta \) and \( S \) alone and behaves independently from types of PSD (as
Figure 2.20: (a) and (b): simulation data of scaled pressure in the quasistatic regime versus the predictions from the models based on $Z_2$ at various volume fractions. The line represents $y = x$. In (a), Hertzian contact is used, and all PSD considered in this study (binary, linear, Gaussian, and lognormal distributions as well as monodisperse particles) are included. In (b), Hookean contact is used, and binary and longormal distributions with $\delta = 0.4$ as well as monodisperse particles are included. In both (a) and (b), $Z_{2c} = 4.26$ is used. (c): $\alpha Z_2$ used in (a) vary for $\delta$, $S$, as well as types of size distributions, as per the legend from Figure 2.19.

shown in Figure 2.19), as shown in Figure 2.20(c), the model constant $\alpha Z_2$ depends on types of PSD. However, within each type of PSD, similar behaviors to those of $\phi_c$ are observed. For a given polydispersity $\delta$, $\alpha Z_2$ increases roughly linearly with increasing $S$. For negative skewness, the polydispersity $\delta$ has weaker impact on $\phi_c$ compared with the case of positive skewness.

### 2.3.5 Shear stress ratio

Same as the first part of this chapter, we model shear stress ratio $\eta \equiv \tau/p$. The following relation proposed by Chialvo et al. [52] for frictional monodisperse particles is used as the basis for study here,

$$\eta(I) = \eta_s(\mu) + \frac{\alpha_1}{(I_0/I)^{\beta_1} + 1}. \quad (2.34)$$

Here, $\eta_s$ is the yield stress ratio, and varies with particle friction coefficient $\mu$ [52].
For particles with binary size distribution, it has been found that the inertial number model is still valid [17, 60, 105]. Furthermore, several studies [60, 105, 110] have found that the yield stress ratio $\eta_s$ is roughly unchanged when particles become polydisperse. In contrast, one study [17] found that $\eta_s$ changes when particles become polydisperse.

In the present study, it is found that the inertial number model is indeed capable of capturing the shear stress ratio $\eta$ for particles with PSD, provided that two changes are made to the original model as in Eqn. (2.34). First, $I$ is defined as $I_{PSD} = \dot{\gamma}d_{43}/\sqrt{\rho/\rho_s}$, to be consistent with the mean diameter choice made for collapsing the pressure data. Second, the yield stress ratio $\eta_s$ no longer depends on $\mu$ alone, but also depends on PSD. As shown in Figure 2.21(d), similar to $\phi_c$ (Figure 2.19), $\eta_s$ is roughly independent from particular type of PSD, and can be described with $\delta$ and $S$ alone. Thus, one can propose an equation to describe $\eta_s$ as done for $\phi_c$ in Eqn. (2.29).

$$\eta_s = \eta_{s_{mono}}(\mu) + c_3(\mu)\delta + c_4(\mu)S\delta^2.$$  (2.35)

For $\mu = 0.5$ here, $\eta_s = 0.382$, $c_3 = 0.0306$, and $c_4 = 0.0563$. Again, for monodisperse particles ($\delta = 0$ and $S = 0$), $\eta_s$ returns to $\eta_{s_{mono}}$, which depends on particle friction coefficient $\mu$ as determined previously [52]. As denoted by the lines in Figure 2.21(d), the equation describes $\eta_s$ reasonably well.

Thus, the stress ratio model Eqn. (2.34) becomes,

$$\eta(I_{43}) = \eta_s(\mu, \delta, S) + \frac{\alpha_1}{(I_0/I_{PSD})^{\beta_1} + 1}.$$  (2.36)

Here, the model constants $\alpha_1$, $\beta_1$, and $I_0$ do not change when particles become polydisperse. It should be noted that the inertial number model by itself is only applicable for hard particles [52]. Also, most granular materials encountered in reality are hard. As shear stress $\dot{\gamma}$ scales with $1/\sqrt{k}$, the intermediate regime is not accessible for hard particles. As shown previously for monodisperse particles [52], a correction is needed for the softness in the in-
termediate regime, which is not explored in the study here. As shown in Figures 2.21(a)(c), this modified inertial number $I_{\text{PSD}}$ collapses the shear stress ratio from various size distributions for both Hertzian and Hookean contacts. In addition, Eqn. (2.36) describes the collapsed data well for both contacts. For high $I_{\text{PSD}}$ values, where lower volume fractions reside (e.g. $\phi = 0.51$), simulation data start to scatter. This behavior is expected; the system enters the collisional regime where kinetic theory describes the behavior well instead [69].

Similar to the pressure behavior in Section 4, replacing volume-averaged diameter $d_{43}$ with Sauter-mean diameter $d_{32}$ would yield an equally decent collapse of shear stress ratio, as shown in Figure 2.21(b). Nonetheless, $d_{43}$ is primarily used for scaling in the study here.

### 2.3.6 Conclusions

We have investigated shear flows of dense, frictional granular materials of various size distributions via DEM simulations. The inertial, quasistatic, and intermediate regimes observed for monodisperse particles persist for polydisperse particles. However, the critical volume fraction that separates the quasistatic and inertial regimes is increased when particles have size distributions. This critical volume fraction is found to be the same for both Hookean and Hertzian contact models, and can be described with fair accuracy by polydispersity $\delta$ and skewness $S$ alone. We further demonstrate that pressure can be scaled by powers of the distance to the jamming volume fraction, in the same manner as was done for the case of uniformly sized particles [52], provided that we recognize that the jamming volume fraction and the effective particle size change with PSD. Furthermore, it is found that the inertial number model for stress ratio is valid for polydispersity, provided that the yield stress ratio is slightly increased when particles manifest size distribution, whose value can be again roughly described by $\delta$ and $S$ alone. Steady-shear rheological models are proposed that capture the simulation results obtained in the simulations for particles with various size distributions.
Figure 2.21: (a-c): shear stress ratio versus inertial number for simulations for particles of various size distributions. Simulations with $\dot{\gamma}$ below $10^{-4}$ are included. Symbols denote simulation results at various volume fractions as per the legend from Figure 2.15. In (a) and (b), Hertzian contact is used, and all PSD considered in this study (binary, linear, Gaussian, and lognormal distributions as well as monodisperse particles) are included. In (c), Hookean contact is used, and binary and lognormal distributions with $\delta = 0.4$ as well as monodisperse particles are included. For scaling, $d_{43}$ is used in (a) and (c), and $d_{32}$ is used in (b). In (a-c), lines denote model predictions from Eqn. (2.36). In (a) and (b), $\alpha_1 = 0.27$, $\beta_1 = 1.0$, and $I_o = 0.2$. In (c), $\alpha_1 = 0.37$, $\beta_1 = 1.5$, and $I_o = 0.2$. (d): $\eta_s$ used in (a-c) vary for $\delta$, $S$, and behave roughly independent from types of size distributions, as per the legend from Figure 2.19. The lines denote the model predictions using Eqn. (2.35), where $\eta_s = 0.382$, $c_3 = 0.0306$, and $c_4 = 0.0563$. 
Based on studies on dense-flow rheology [52], kinetic theory has been modified to take account of friction and dense regime [28, 29]. It would be interesting to modify recently developed kinetic theory for polydisperse particles (e.g., [102, 103]) using the results of the present study to account for friction and dense regime. This would then yield a dynamic stress model for frictional granular materials with any size distribution.
Chapter 3

Development and validation of CFD-DEM approach for cohesive particles

Overview of the chapter

This chapter has two parts. We first develop a CFD-DEM approach that appropriately accounts for interparticle cohesion; we then use the developed method to study a specific problem and compare with the experimental results to validate the method.

- In the first part, we focus on developing a CFD-DEM approach that appropriately accounts for cohesion. CFD-DEM simulations are performed to study gas-fluidization of particles with van der Waals force cohesion for both Group A and Group C particles. The particle spring constant used in such CFD-DEM simulations is commonly much smaller than that for realistic particles used in experiments. For cohesive particles,

---

the predicted flow patterns depend on the value of particle spring stiffness used in the simulations. This dependence can be explained through a simple analysis involving head-on collision of two particles. A modified cohesion model is then proposed and verified through simulations of two-particle collisions. Simulations of gas-fluidization of cohesive particles with this modified cohesion model reveal that the predicted distributions of bubble size are insensitive to particle stiffness for Group A particles. For Group C particles, except for substantially small particle stiffness, the flow patterns are preserved when smaller particle stiffness is used.

- In the second part, we apply the modified cohesion model developed in the first part to study the effects of fines (particles with $d_p < 45\mu m$) on fluidization. It is well known that addition of fines improves quality of fluidization [1,2]. However, the mechanism through which the fines affect fluidization quality is not fully understood. Addition of fines not only introduces particle size distribution, but also makes the system more cohesive. It is unclear which property of fines is responsible for its beneficial effect. Here, we probe this question through CFD-DEM simulations. We have performed the simulations of gas-fluidization of Group A particles containing different levels of fines in small periodic domains using ambient air as the fluidizing gas and at various particle volume fractions. Inhomogeneous microstructures that take the form of clusters or bubble-like voids readily form when no fines were added. Introducing fines did not lead to appreciable improvement in the quality of fluidization, when van der Waals force of interaction between particles was not included. In contrast, the addition of cohesion due to van der Waals force produced significant changes under some flow conditions. At high volume fractions of the base Group A particles, the addition of a small amount of fines was found to be sufficient to eliminate the inhomogeneous microstructure almost completely. The amount of fines required to homogenize the flow increased with decreasing volume fraction of the large particles. This behavior
is found to be consistent with previous experiments, which validate the simulation approach.

3.1 Development of a modified cohesion model to be used in CFD-DEM simulations

3.1.1 Introduction

CFD-DEM simulations have been used to study and explain the effects of cohesion on fluidization of particles [111–115]. To accelerate simulations, all the studies mentioned above have adopted small spring constants to allow for larger DEM time steps. They are based on the assumption that the flow patterns would not be altered with smaller spring constants. Indeed, for non-cohesive particles, it has been shown that the flow patterns in CFD-DEM simulations are insensitive to spring constants [15]. However, for cohesive particles, it has been clearly shown that the spring stiffness does affect flow behaviors in fluidization of cohesive particles [116]. Recently, Kobayashi et al. [117] studied fluidization of particles which exhibit attractive interactions while they are in contact with each other, and proposed how one could modify the cohesion model, so that the simulations with softer spring constants would yield similar results as those with realistic spring constants.

In the present study, CFD-DEM simulations are performed on gas-fluidization of particles for both non-cohesive and particles with van der Waals force cohesion. We consider in our analysis mildly cohesive Geldart group A particles which exhibit a window of bubble-less bed expansion after minimization fluidization as well as strongly cohesive group C particles that are difficult to fluidize [9]. It is found that, when softer particles are used, flow patterns are not changed for non-cohesive particles, but are altered substantially for cohesive particles. To mitigate this dependence, a modified cohesion model is proposed, verified through simu-
lations of two-particle collision, and then applied to gas-fluidization simulations. It is found that for Group A particles, flow patterns are essentially insensitive to particle stiffness, in a statistical sense. For Group C particles, except for substantially small particle stiffness, the flow patterns are preserved when smaller particle stiffness is used.

There are two notable differences between the work by Kobayashi et al. [117] and the one proposed here. Contrary to the study by Kobayashi et al. [117], the proposed modified cohesion model takes account of the van der Waals force even when particles are not in contact. Further, the model proposed by Kobayashi et al. [117] is limited to Hookean contact model, while we propose modifications to the van der Waals force model for both Hookean and Hertzian contact models.

### 3.1.2 Simulation methodology

We model the gas phase using Computational Fluid Dynamics via an OpenFOAM-based solver [118], and solid phase using Discrete Element Method [53] via LIGGGHTS [119]. The two phases are coupled via CFDEMcoupling [120].

Particle motion is followed by solving Newton’s equations of motion:

\[
m_i \frac{dv_i}{dt} = \sum_j (f_{c,ij}^n + f_{c,ij}^t) + \sum_k f_{v,ik} + \sum_w (f_{c,iw}^n + f_{c,iw}^t + f_{v,iw}) + f_{g-p,i} + m_i g \tag{3.1}
\]

\[
I_i \frac{d\omega_i}{dt} = \sum_j T_{t,ij} + \sum_w T_{t,iw} \tag{3.2}
\]

In the equations, particle \( i \) has mass \( m_i \), moment of inertia \( I_i \), translational and rotational velocities \( \mathbf{v}_i \) and \( \omega_i \). The forces acting on the particle \( i \) are: \( f_{c,ij}^n \) and \( f_{c,ij}^t \) which are the normal and tangential contact forces from the collision of two particles \( i \) and \( j \), \( f_{c,iw}^n \) and \( f_{c,iw}^t \) which are the normal and tangential contact forces from the collision between particle \( i \) and wall, \( f_{v,ik} \) and \( f_{v,iw} \) which are the van der Waals forces from the interactions between two
particles \( i \) and \( k \) and between particle \( i \) and wall, \( f_{g-p,i} \) which is the total interaction force on the particle \( i \) due to surrounding gas (explained further below), and the gravitational force \( m_i g \). The torque acting on particle \( i \) due to particle \( j \) is \( T_{t,ij} \), which results from the tangential force. \( T_{t,ij} = R_{ij} \times f_{t,ij} \), where \( R_{ij} \) is the vector from the center of particle \( i \) to the contact point. \( T_{t,iw} \) is the torque acting on particle \( i \) from wall. Rolling friction is not accounted for in the present simulations.

The particle contact forces \( f_{c,ij}^n \) and \( f_{c,ij}^t \) are calculated using a Hookean (linear) or Hertzian contact model. For linear contact (spring–dashpot) model,

\[
f_{c,ij}^n = k_n \delta_n n_{ij} - \gamma_n m^* v_{ij}^n, \quad (3.3)
\]

\[
f_{c,ij}^t = \begin{cases} k_t t_{ij} - \gamma_t m^* v_{ij}^t & \text{for } |f_{c,ij}^t| < \mu_s |f_{c,ij}^n| \\ -\mu_s f_{c,ij}^n \frac{t_{ij}}{|t_{ij}|} & \text{for } |f_{c,ij}^t| \geq \mu_s |f_{c,ij}^n| \end{cases}, \quad (3.4)
\]

The subscripts \( i, j \) denote spherical particle \( i \) or \( j \), and the superscript * denotes the effective particle property of those two particles. The effective particle mass \( m^* \) is calculated as \( m^* = m_i m_j / (m_i + m_j) \), \( k_n \) and \( k_t \) are spring elastic constants, and \( \gamma_n \) and \( \gamma_t \) are viscous damping coefficients, \( \delta_n \) is normal overlap distance, \( n_{ij} \) represents the unit normal vector pointing from particle \( i \) to particle \( j \), \( v_{ij}^n \) represents the relative normal velocity of particles \( i \) and \( j \), \( t_{ij} \) represents the tangential displacement obtained from the integration of the relative tangential velocity during the contact, \( v_{ij}^t \) represents the relative tangential velocity of particles \( i \) and \( j \), \( \mu_s \) is the particle sliding friction coefficient. As used in simulations by Tsuji et al. [15], in our simulations, \( k_n = k_t \) (referred as \( k \) in the rest of study here), and \( \gamma_n = \gamma_t \). \( \gamma_n \) is calculated based the model input of the restitution coefficient \( e \): 

\[
e = \exp\left( -\frac{\gamma_n \pi}{\sqrt{4k_n m^* - \gamma_n^2}} \right).
\]
For Hertzian contact model, $f_{c,ij}^n$ and $f_{c,ij}^t$ are calculated by the following [121, 122]:

\[
f_{c,ij}^n = \frac{4}{3} Y^* \sqrt{r^*} \delta_{ni} n_{ij} + 2 \sqrt{\frac{5}{6}} \beta \sqrt{S_n m^*} v_{ij}^n, \tag{3.5}
\]

\[
f_{c,ij}^t = \begin{cases} 
8 G^* \sqrt{r^*} \delta_{nt} t_{ij} + 2 \sqrt{\frac{5}{6}} \beta \sqrt{S_t m^*} v_{ij}^t & \text{for } |f_{c,ij}^t| < \mu_s |f_{c,ij}^n| \\
-\mu_s |f_{c,ij}^n| t_{ij} & \text{for } |f_{c,ij}^t| \geq \mu_s |f_{c,ij}^n|, 
\end{cases} \tag{3.6}
\]

where

\[
\frac{1}{Y^*} = \frac{1 - \nu_i^2}{Y_i} + \frac{1 - \nu_j^2}{Y_j}, \quad \frac{1}{r^*} = \frac{1}{r_i} + \frac{1}{r_j}, \tag{3.7}
\]

\[
\beta = \frac{\ln(e)}{\sqrt{\ln^2(e) + \pi^2}}; \quad S_n = 2 Y^* \sqrt{r^*} \delta_n, \tag{3.8}
\]

\[
\frac{1}{G^*} = \frac{2(2 + \nu_i)(1 - \nu_i)}{Y_i} + \frac{2(2 + \nu_j)(1 - \nu_j)}{Y_j}, \quad S_t = 8 G^* \sqrt{r^*} \delta_n. \tag{3.9}
\]

Here, $Y$ is Young’s modulus, $G$ is shear modulus, $\nu$ is Poisson’s ratio, and $r$ is particle radius.

Eqns. (3.3) and (3.4) for Hookean contact model and Eqns. (3.5) and (3.6) for Hertzian contact model can be used to model particle contact forces between a particle and wall, $f_{c,iw}^n$ and $f_{c,iw}^t$. The only difference is that particle $j$ is now treated as a particle with infinite radius, and thus $m^* = m_j$.

The magnitude of van der Waals force $F_{vdw}$ between particles $i$ and $k$ is modeled by the following [112, 123]:

\[
F_{vdw}(A, s) = A \frac{2r_i r_j (r_i + r_k + s)}{3 s^2 (2r_i + 2r_k + s)^2} \left[ \frac{s(2r_i + 2r_k + s)}{(r_i + r_k + s)^2 - (r_i - r_k)^2} - 1 \right]^2, \tag{3.10}
\]

where $A$ is the Hamaker constant which depends on the material properties [124], and $s$ is the distance between the particle surfaces. It is assumed that the force saturates at a minimum separation distance, $s_{min}$ (corresponding to the inter-molecular spacing) [56]. This constant maximum force is also applied when the particles are in contact. Since the magnitude of
the van der Waals force quickly decreases as the distance between the surfaces increases, a
maximum cutoff distance \( s_{\text{max}} = (r_i + r_j)/4 \) [57] is used to accelerate the simulation. For
\( s > s_{\text{max}} \), the van der Waals force is not accounted for. As illustrated by the thick solid lines
in Figure 3.1 for the case of \( A = A^R \) and \( s_{\text{min}} = s_{\text{R min}}^R \), the van der Waals force \( f_{v,ik} \) between
particles \( i \) and \( k \) can now be modeled as,

\[
f_{v,ik} = -f_{v,ik}n_{ik} = \begin{cases} 
-F_{vdw}(A, s)n_{ik} & \text{for } s_{\text{min}} < s < s_{\text{max}} \\
-F_{vdw}(A, s_{\text{min}})n_{ik} & \text{for } s \leq s_{\text{min}} 
\end{cases}
\] (3.11)

In the limit that \( s \) becomes much smaller than the particle radii, the expression for \( F_{vdw} \)
(Eqn. (3.10)) can be reduced to the more familiar expression: \( F_{vdw} = \frac{A'r_p}{12\pi} \). It is found that
the magnitude of van der Waals force between a particle \( i \) and a flat surface (e.g. wall) \( F_{vdw,w} \) is effectively twice of it: \( F_{vdw,w} = \frac{A'r_p}{6\pi} \) [112, 123, 124]. Thus, the van der Waals force
\( f_{v,iw} \) between particle \( i \) and wall experience by particle \( i \) can now be modeled as,

\[
f_{v,iw} = -f_{v,iw}n_{iw} = \begin{cases} 
-\frac{A'r_p}{6\pi}n_{iw} & \text{for } s_{\text{min}} < s < s_{\text{max}} \equiv r_i/4 \\
-\frac{A'r_p}{6s_{\text{min}}}n_{iw} & \text{for } s \leq s_{\text{min}} 
\end{cases}
\] (3.12)

The fluid phase is modeled by solving the following conservation of mass and momentum
equations in terms of the locally averaged variables over a computational cell:

\[
\frac{\partial}{\partial t}(1 - \phi) + \nabla \cdot [(1 - \phi)\mathbf{u}] = 0,
\] (3.13)

\[
\rho_g(1 - \phi) \left( \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p_g + \nabla \cdot \mathbf{\tau}_g + \Phi_d + \rho_g(1 - \phi)\mathbf{g}.
\] (3.14)

Here, \( \rho_g \) is the density of the gas and assumed to be constant, \( \phi \) is the solid volume fraction,
\( \mathbf{u} \) is the gas velocity, \( p_g \) is the gas phase pressure, \( \mathbf{\tau}_g \) is the gas phase deviatoric stress tensor.
The total gas-particle interaction force per unit volume of the mixture \( -\Phi_d \), exerted on the
particles by the gas, is composed of a generalized buoyancy force due to the slowly-varying
Figure 3.1: Schematic of the original (Eqn. (3.11)) and modified (Eqn. (3.20)) cohesion models between two particles.
(in space) local-average gas phase stress \((-p_g I + \tau_g)\) and the force due to the rapidly varying flow (in space) field around the particles. \(\Phi_d\) is related to \(f_{g\to p,i}\) as \(\Phi_d = \sum_i f_{g\to p,i}; \Phi_d\) is the summation of \(f_{g\to p,i}\) for all the particles in the computational cell. On a per particle basis, the total interaction force on the particle by the gas can be written as \(f_{g\to p,i} = -V_{p,i}\nabla p_g(x = x_{p,i}) + V_{p,i}\nabla \cdot \tau_g(x = x_{p,i}) + f_{d,i}\), where \(V_{p,i}\) is the particle volume and \(f_{d,i}\) is the gas-particle force due to fluid flow around the particle. Subscript \(i\) indicates that quantities are per particle, and that fluid phase properties have been interpolated at the particle position. In this study, we only consider the drag force, which is the most important component of \(f_{d,i}\) for gas-particle flows, and use the Wen and Yu [51] drag law. As \(\tau_g\) is relatively insignificant in \(f_{g\to p,i}\) for modeling gas-fluidized beds of particles, the term is not accounted for in modeling \(f_{g\to p,i}\).

### 3.1.3 Simulation conditions

We perform simulations of gas-fluidization of both non-cohesive and cohesive particles in a geometry similar to the one in the experiments by Kobayashi et al. [117]. However, due to the limitation in computations for the cases of high spring stiffness, as well as the fact that the objective of this study here is to investigate the effects of spring stiffness on fluidization behaviors, a much smaller domain is simulated. The computation domain and its boundary conditions are illustrated in Figure 3.2.

The simulation parameters are given in Table 3.1. Material properties for the particles are taken from the literature [111, 117]. As shown in Table 3.1, several values for Young’s modulus \((Y)\) are used, and \(Y = 7 \times 10^{10} Pa\) represents a typical Young’s modulus of the particles [117]. Several values for linear spring constants \((k)\) are used, and it has been found [117] that \(k = 7000 N/m\) corresponds to the typical material properties of particles: \(Y = 7 \times 10^{10} Pa\) and \(\nu = 0.22\). Two Hamaker constants \((A)\) are chosen to represent Group A and Group C particles. Molerus [49] suggested that accounting for interparticle cohesive
forces results in a classification of powders which is equivalent to the one by Geldart [9] that is based on density difference and mean particle size. Specifically, ratio between interparticle cohesive force and particle weight can be used to distinguish different groups [49, 125]. With this in mind, we simulate fluidization of assemblies of identical particles for different values of the Bond number (Bo), which is the ratio of the maximum cohesive force between two particles and the particle weight. For Group A particles, interparticle cohesive force and particle weight are of comparable magnitudes [49, 125], or $Bo \approx 1$. For Group C particles, interparticle cohesive force suppresses free particle motion [49], and $Bo \geq 10$ [114]. Correspondingly, $A = 2.1 \times 10^{-21} J$ is used in this study to yield $Bo = 2$ to represent Group A particles, and $A = 4.2 \times 10^{-20} J$ is used to yield $Bo = 42$ to represent Group C particles.

DEM time step $t_{DEM}$ must be sufficiently small compared to collision time $t_{coll}$ to resolve the particle collisions. $t_{DEM} = t_{coll}/50$ [126] is used. For Hookean contact model, $t_{coll}$ is found by $t_{coll} = \pi(2k_n/m - \gamma_n^2/4)^{-1/2}$ [126], where $m$ is the mass of a particle. For Hertzian contact
model, \( t_{\text{coll}} \) is found by \( t_{\text{coll}} = 2.943 \left( \frac{5\sqrt{2\pi} (1-\nu^2)}{4Y} \right)^{2/5} \frac{R}{\nu_0^{4/5}} \). \cite{117, 127}. \( t_{\text{coll}} \) depends on the normal approaching velocity of the particle \( v_o \). \( v_o = 0.002 \, \text{m/s} \) is found to be the average colliding velocity for the system studied here \cite{117}, and is thus used to calculate \( t_{\text{coll}} \). \( t_{\text{coll}} \) and \( t_{\text{DEM}} \) values for different cases considered here are summarized in Table 3.2.

At the beginning of each simulation, a fixed number of particles are randomly generated without overlaps. The particles are allowed to settle due to gravity. The settling process is continued until velocities of particles decrease essentially to zero. Consistent with the experiments \cite{117}, the gas is uniformly injected at the bottom at the superficial velocity \( u_f \) of 0.02 m/s.

Table 3.1: Parameter values used in the simulations.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Geometry of container; width \times depth \times height (mm)</td>
<td>3 \times 0.18 \times 7.65</td>
</tr>
<tr>
<td>Acceleration due to gravity; g (m/s(^2))</td>
<td>9.81</td>
</tr>
<tr>
<td>Number of particles;</td>
<td>9522</td>
</tr>
<tr>
<td>Particle diameter; ( d_p ) (( \mu )m)</td>
<td>60</td>
</tr>
<tr>
<td>Particle density; ( \rho_p ) (kg/m(^3))</td>
<td>2250</td>
</tr>
<tr>
<td>Young’s modulus; ( Y ) (Pa)</td>
<td>7 \times 10^{10}, 10^8, 10^6</td>
</tr>
<tr>
<td>Poisson’s ratio; ( \nu )</td>
<td>0.22</td>
</tr>
<tr>
<td>Linear spring constant; ( k ) (N/m)</td>
<td>7000, 100, 10</td>
</tr>
<tr>
<td>Restitution coefficient; ( e )</td>
<td>0.94</td>
</tr>
<tr>
<td>Sliding friction coefficient; ( \mu_s )</td>
<td>0.18</td>
</tr>
<tr>
<td>Hamaker constant; ( A ) (J)</td>
<td>2.1 \times 10^{-21}, 4.2 \times 10^{-20}</td>
</tr>
<tr>
<td>Minimum separation distance; ( s_{\text{min}} ) (nm)</td>
<td>1</td>
</tr>
<tr>
<td>Gas density; ( \rho_g ) (kg/m(^3))</td>
<td>1.205</td>
</tr>
<tr>
<td>Gas kinematic viscosity; ( \mu_g ) (Pa \cdot s)</td>
<td>1.81 \times 10^{-5}</td>
</tr>
<tr>
<td>Superficial gas velocity; ( u_f ) (m/s)</td>
<td>0.02</td>
</tr>
<tr>
<td>Cell size for fluid flow; width \times depth \times height (mm)</td>
<td>0.18 \times 0.18 \times 0.18</td>
</tr>
</tbody>
</table>

Table 3.2: DEM time steps employed for simulations.

<table>
<thead>
<tr>
<th>( t_{\text{coll}} ) ( (t_{\text{coll}}/50) )</th>
<th>Hookean contact model, ( k ) (N/m)</th>
<th>Hertzian contact model, ( Y ) (Pa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 7000 )</td>
<td>4.2 \times 10^{-7}</td>
<td>7 \times 10^{10}</td>
</tr>
<tr>
<td>( 100 )</td>
<td>3.5 \times 10^{-6}</td>
<td>10^8</td>
</tr>
<tr>
<td>( 10 )</td>
<td>1.1 \times 10^{-5}</td>
<td>10^6</td>
</tr>
<tr>
<td>( 7 \times 10^{-6} )</td>
<td>6.0 \times 10^{-7}</td>
<td>1 \times 10^{-8}</td>
</tr>
<tr>
<td>( 1 \times 10^{-6} )</td>
<td>8.2 \times 10^{-6}</td>
<td>1.5 \times 10^{-7}</td>
</tr>
<tr>
<td>( 1 \times 10^{-7} )</td>
<td>5.2 \times 10^{-5}</td>
<td>( 1 \times 10^{-6} )</td>
</tr>
</tbody>
</table>
3.1.4 Results and discussions

Non-cohesive particles

As mentioned before, it has been shown [15] that the flow patterns are insensitive to spring softness for non-cohesive particles. Here, we present simulation results to confirm this observation. During simulations, domain-average slip velocity in the vertical direction increases and then fluctuates around a fixed value after around 0.1 s, indicating that the system has reached a steady state (in a time-averaged sense). The domain-average slip velocity is defined as the difference between the Favre-average gas velocity in the domain and the average velocity of all the particles. Several snapshots at different time steps at steady state (taken after 0.2 s) for Hookean contact model with different $k$ values are shown in Figure 3.3. As shown in the figures, decreasing $k$ slightly increases the coordination number $Z$ in the system, which is expected since particles would on average spend more time in collision when the spring becomes softer. However, the general flow patterns seem preserved, as bubbles have similar shapes and sizes.

To quantify the effect of spring softness on the flow patterns in the system, bubble/crack distribution is studied. Following the analysis by Kobayashi et al. [117], a bubble/crack is defined as a closed domain whose components (CFD cells) have voidage larger than 0.8. Bubble diameter is defined as the diameter of a sphere having the same volume of the bubble. Particle analysis function in ImageJ, an image processing program developed at the National Institute of Health, USA, is used to analyze snapshots of voidage distribution at steady state (from 0.2 s to 1 s), to obtain the distribution of bubbles (cracks). The results are presented in Figure 3.4(a), where the cumulative volume fraction of bubble diameter is plotted. As shown in the figure, the distributions of bubble sizes for different $k$ values are very similar.

Similar results were obtained for non-cohesive particles using Hertzian contact model as well. Representative snapshots at “statistical” steady state for different $Y$ values are presented
Figure 3.3: Snapshots of fluidization of non-cohesive particles for Hookean contact model with different $k$ values at several time steps at steady state. Similar flow patterns are observed for different $k$ values.
Figure 3.4: Cumulative volume fraction of bubbles versus bubble diameter for both Hookean and Hertzian contacts. Particles are non-cohesive. Bubble size distribution is found insensitive to spring stiffness for both contact models.

in Figure 3.5. Cumulative volume fraction of bubble diameters is included in Figure 3.4(b). Both bubble shapes and bubble size distributions are shown to be insensitive to $Y$ values. Thus, simulations employing both Hookean and Hertzian contacts confirm the observations that, flow patterns are insensitive to spring stiffness for non-cohesive particles.

Figure 3.5: Representative snapshots of fluidization of non-cohesive particles for Hertzian contact model with different $Y$ values at several time steps at steady state. Similar flow patterns are observed for different $Y$ values.
Cohesive particles with the original cohesion model

Similar analysis is performed when the van der Waals force models described in Eqns. (3.11) and (3.12) are included. \( A = 2.1 \times 10^{-21} \) corresponding to Group A particles is first considered. Snapshots taken at different times (in the statistical steady state) for Hookean contact model with different \( k \) values are shown in Figure 3.6 (rows 1, 2, and 4 for \( k \) of 7000 \( N/m \), 100 \( N/m \), and 10 \( N/m \), respectively). As shown in the figure, when softer springs are used, two notable changes are made to the flow patterns: (1) large agglomerates characterized by large coordination number \((Z > 5)\) spanning the entire width of the simulation domain are formed. (2) Instead of bubbles, small cracks are formed. The cumulative volume fraction of bubble diameter, shown in Figure 3.7(a) confirms these changes to the flow patterns, as the curve is shifted to the left, corresponding to the replacement of bubbles with small cracks observed in the snapshots.

Similar results are obtained for Group A particles with Hertzian contact. Representative snapshots in the statistical steady state for different \( Y \) values are presented in Figure 3.8. When soft springs are used, large agglomerates spanning the width of the simulation domain form; and, cracks, instead of bubbles are predicted. Cumulative volume fraction of bubble diameters is included in Figure 3.7(b). When softer spring is used, the curve is shifted to the left.

These drastic effects of spring stiffness on flow patterns are even more pronounced when Group C particles \((A = 4.2 \times 10^{-20} \) \) are considered. Several snapshots at different time steps during initial fluidization period are shown in Figure 3.9 (rows 1, 2, and 4 for \( k \) of 7000 \( N/m \), 100 \( N/m \), and 10 \( N/m \), respectively). As shown in the figure, for the real linear spring constant \( k = 7000 \) \( N/m \), a crack is initially formed at the bottom of the bed. Then, the crack travels up through the bed. With softer springs \((k \) is 100 \( N/m \) or 10 \( N/m \)), a crack
Figure 3.6: Snapshots of fluidization of cohesive particles for Hookean contact model with different $k$ values at several time steps at steady state. $A = 2.1 \times 10^{-21} J$ is used, which corresponds to Group A particles. Compared with the real linear spring constant $k = 7000 N/m$, smaller spring constants using original cohesion model (Eqns 3.11 and 3.12) yield different flow patterns, whereas ones using modified cohesion model (Eqns 3.20 and 3.26) yield similar flow patterns.
Figure 3.7: Cumulative volume fraction of bubbles versus bubble diameter for both Hookean and Hertzian contacts. Particles are Group A particles, with \( A = 2.1 \times 10^{-21} \text{ J} \). For both contact models, when softer spring is used, bubble size distribution is changed when original cohesion model (Eqns. 3.11 and 3.12) are used, and preserved when modified cohesion model (Eqns 3.20 and 3.26) are used.

Figure 3.8: Representative snapshots of fluidization of cohesive particles for Hertzian contact models with different \( Y \) values at several time steps at steady state. Particles are Group A particles, with \( A = 2.1 \times 10^{-21} \text{ J} \). Compared with the real Young’s modulus \( Y = 7 \times 10^{10} \text{ J} \), smaller spring constants using original cohesion model (Eqns 3.11 and 3.12) yield different flow patterns, whereas ones using modified cohesion model (Eqns 3.20 and 3.26) yield similar flow patterns.
is formed at the beginning of the simulation. This crack is then stuck at the bottom of the bed, as the whole system appears frozen.

Theoretical analysis

The analysis on flow patterns in fluidization of both Group A and Group C particles indicates that using a softer spring substantially changes the flow patterns. Specifically, the simulation results suggest that employing a softer spring enables cohesion to have a greater impact on the flow behaviors. The reasons for this phenomenon can be understood by considering a head-on collision between two identical particles with mass $m_p$. Both particles have equal but opposite normal impact velocities of $v_i$. After collisions, both particles would acquire equal but opposite velocities of $v_o$. The effective restitution coefficient $e_{\text{eff}}$ can be thus calculated as $v_o/v_i$. This collision is performed for various values of $v_i$, and the corresponding $e_{\text{eff}}$ is calculated. The results are plotted in Figure 3.10 (a) for various spring constants as denoted by the legends. Hamaker constant $A$ of $4.2 \times 10^{-20} J$ is used here for illustration. Similar results can be found for other values for $A$. The other particle properties used in the simulations are the same as those that are used before (Table 3.1).

The shape of the curve for each spring constant is consistent with the experimental observations [128, 129]. In the experiments, microspheres with different velocities normal to the surface impact with a flat surface, and the incoming and rebounding particle velocities are measured to calculate the corresponding restitution coefficient. In both the experiments and simulations here, there is a critical velocity $v_c$, below which the two particles would not bounce back, but instead stick to each other. For normal impact velocities larger but close to $v_c$, the effective restitution coefficient has a steep increase as the normal impact velocity increases. As the normal impact velocity further increases, the effective restitution coefficient increases slowly and eventually reaches an asymptote, which equals to the one for non-cohesive particle collision.
Figure 3.9: Snapshots of fluidization of cohesive particles for Hookean contact model with different $k$ values at several time steps during the initial fluidization period. $A = 4.2 \times 10^{-20} J$ is used, which corresponds to Group C particles. Compared with the real linear spring constant $k = 7000 N/m$, smaller spring constants using original cohesion model (Eqns 3.11 and 3.12) yield different flow patterns. Softer spring of $k = 100 N/m$ using modified cohesion model (Eqns 3.20 and 3.26) yields similar flow patterns, although softer spring of $k = 10 N/m$ does not so.
Figure 3.10: Effective restitution coefficients versus impact velocities for various spring constants as per the legend. In (a), the original van der Waals force model (Eqns (3.11)) is used. In (b), only the part of model where particles are in contact is modified (Eqns (3.19)). In (c), the full modified van der Waals force model (Eqns (3.20)). The curve in (c) represents the model prediction from Eqn. (3.25) with $l_c = 1.25 \times 10^{-10}$ m.

However, as shown in Figure 3.10 (a), the dependence of $e_{\text{eff}}$ on $v_i$ is altered when a different spring constant is used. Specifically, as the softer spring constant is used, $v_c$ increases. For a wide range of normal impact velocities, $e_{\text{eff}}$ is reduced when softer spring constant is used. In other words, when softer spring constants are used, the effects of cohesion are more pronounced as particles have more chances to lose kinetic energy and not bounce back.

The reason why softer spring increases $v_c$ and reduces $e_{\text{eff}}$ can be easily understood. The van der Waals force $f_{v,ik}$ (Eqn. (3.11)) can be decomposed into two components: $f_{v1,ik}$, which is present when particles do not overlap ($s > 0$), and $f_{v2,ik}$, which is constant ($= F_{vdw}(A,s_{\text{min}})$) and present when particles overlap ($s < 0$). When softer spring is used instead of the real spring, the particles would overlap more. As a result, even though the work done by $f_{v1,ik}$, $W_{v1}$, is unaffected, work done by $f_{v2,ik}$, $W_{v2} = f_{v2,ik} l_{v2}$, is increased as it is applied over larger distance for softer spring ($l^S_{v2}$) than for real spring ($l^R_{v2}$). Thus, to preserve $W_{v2}$ when softer spring is used, or $W^S_{v2} = W^R_{v2}$, one needs to adjust $f_{v2,ik}$ appropriately: $f^S_{v2,ik} l^S_{v2} = f^R_{v2,ik} l^R_{v2}$, or $f^S_{v2,ik} = f^R_{v2,ik} l^R_{v2} / l^S_{v2}$. The total distance $l_{v2}$ over which $f_{v2,ik}$ is applied is the maximum
overlap distance $\delta_{\text{max}}$. Thus, the following relationship is established:

$$f^S_{v_2,ik} = f^R_{v_2,ik} \delta^R_{\text{max}}/\delta^S_{\text{max}}.$$  (3.15)

As $f_{v_2,ik}$ or $F_{vdw}(A, s_{\text{min}})$ is linear proportional to Hamaker constant $A$, as shown in Eqn (3.10), Eqn. (3.15) can be written as

$$A^S = A^R \delta^R_{\text{max}}/\delta^S_{\text{max}}.$$  (3.16)

Now, one seeks to relate $\delta_{\text{max}}$ to $k$ in the case of Hookean contact model or $Y$ in the case of Hertzian contact model. When particles reach the maximum overlap distance, all the initial kinetic energy $E_k = m_p v_i^2$ is converted to potential energy $E_v$, and energy loss due to viscous damping and cohesion. For problems considered in this study, essentially all the initial kinetic energy is converted to potential energy. For example, $E_v/E_k$ is 99.18% for the normal impact velocities of 0.005 m/s for Hookean contact model. Thus, for Hookean contact model, when the real spring constant $k_R$ is replaced by a softer spring constant $k_S$, the potential energy $E_p$ at $\delta_{\text{max}}$ remains essentially constant and equal to $E_k$. In other words, $1/2k_R \delta^R_{\text{max}}^2 = E_k = 1/2k_S \delta^S_{\text{max}}^2$, or $\delta^R_{\text{max}}/\delta^S_{\text{max}} = (k_S/k_R)^{1/2}$. Thus, together with Eqn. (3.16), we obtain the following:

$$A^S = A^R(k_S/k_R)^{1/2}.$$  (3.17)

The exponent of 1/2 coincides with the finding by Kobayashi et al. [117], whose analysis is based on solving the differential equation for the collision between a particle and a wall.

Similarly, for the Hertzian contact model, when the real Young’s modulus $Y_R$ is replaced by a softer one $Y_S$, the potential energy energy $E_p$ essentially remains to $E_k$. Thus, $Y_R \delta^R_{\text{max}}^{5/2} = \ldots$
\[ Y_S\delta_{\text{max}}^{5/2}, \text{ and } \delta_{\text{max}}^{R}/\delta_{\text{max}}^{S} = (Y_S/Y_R)^{2/5}. \] With Eqn. (3.16), we obtain the following:

\[ A^S = A^R(Y_S/Y_R)^{2/5}. \] (3.18)

Eqns. (3.17) and (3.18), for Hookean and Hertzian contacts respectively, can be used for \( f_{v2,ik} \), with \( f_{v1,ik} \) unchanged, so that the total work done by \( f_{v,ik} \) is preserved when softer spring is used. Thus, a new cohesion model \( f'_{v,ik} \) is proposed:

\[
f'_{v,ik} = -f'_{v,ik}n_{ik} = \begin{cases} 
-F_{\text{vdw}}(A^R, s)n_{ik} & \text{for } s_{\text{min}} < s < s_{\text{max}} \\
-F_{\text{vdw}}(A^R, s_{\text{min}})n_{ik} & \text{for } 0 < s \leq s_{\text{min}} \\
-F_{\text{vdw}}(A^S, s_{\text{min}})n_{ik} & \text{for } s \leq 0,
\end{cases}
\] (3.19)

where \( A^S \) is calculated by Eqns. (3.17) and (3.18) for Hookean and Hertzian contacts, respectively.

However, as shown in Figure 3.10 (b), even though the curves for different spring constants are brought closer with this correction, the data points for softer springs are rather scattered in the region where \( e_{\text{eff}} \) sharply increases with increasing \( u_i \). It is due to the large difference in \( f'_{v,ik} \) near \( s = 0 \), as \( \lim_{x \to 0^-} f'_{v,ik} = F_{\text{vdw}}(A^S, s_{\text{min}}) \) is much smaller than \( \lim_{x \to 0^+} f'_{v,ik} = F_{\text{vdw}}(A^R, s_{\text{min}}) \). As a result, when the particles come to contact, \( f_{v,ik} \) might be over-estimated, and when the particles come out of contact, \( f_{v,ik} \) might be under-estimated. Thus, \( e_{\text{eff}} \) can be either over-estimated or under-estimated, causing scattering. It is found that if a much smaller time step is used, this scattering would disappear. However, that scenario is undesirable, as the reason for using softer springs is to allow for larger time steps to accelerate simulations.

To address this issue, a new modified van der Waals force model is developed, as illustrated in the thick dashed line in Figure 3.1 (the thick solid line represents the original model). In
this new model, the same modification is applied to $f_{v2,ik}$. However, there are two changes on $f_{v1,ik}$: (1) $f_{v1,ik}$ is shifted to the right side by $s_o$. (2) The minimum separation distance, $s_{\text{min}}$ at which $f_{v1,ik}$ saturates is increased from $s_{\text{Rmin}}$ to $s_{\text{Smin}}$. Thus, a new modified cohesion model $f_{v,ik}^M$ is proposed:

$$f_{v,ik}^M = -f_{v,ik}^M n_{ik} = \begin{cases} -F_{vdw}(A^R, s - s_o) n_{ik} & \text{for } s_{\text{Smin}} < s < s_{\text{max}} \\ -F_{vdw}(A^S, s_{\text{Smin}}) n_{ik} & \text{for } s \leq s_{\text{Smin}}, \end{cases}$$  \hspace{1cm} (3.20)

where $s_o$ and $s_{\text{Smin}}$ are subjected to the following constraints:

$$F_{vdw}(A^S, s_{\text{Smin}}) = F_{vdw}(A^R, s_{\text{Smin}} - s_o) \hspace{1cm} (3.21)$$

$$F_{vdw}(A^R, s_{\text{Rmin}}) \cdot s_{\text{Rmin}} + \int_{s_{\text{Rmin}}}^{s_{\text{Smax}}} F_{vdw}(A^R, s) ds = F_{vdw}(A^S, s_{\text{Smin}}) \cdot s_{\text{Smin}} + \int_{s_{\text{Smin}}}^{s_{\text{Smax}}} F_{vdw}(A^R, s - s_o) ds.$$  \hspace{1cm} (3.22)

These modification to the model are made to achieve the three objectives: (1) The new van der Waals force model would not experience a sharp change in magnitude near $s = 0$. (2) In the new van der Waals force model, the work done by $f_{v1,ik}$ is preserved. (3) In the new van der Waals force model, the dependence of $f_{v1,ik}$ on $s$ should be similar to the original one.

Eqn. (3.17) for Hookean contact model or Eqn. (3.18) for Hertzian contact model is used to simplify Eqns. (3.21) and (3.22) to the following:

$$F_{vdw}(\theta, s_{\text{Smin}}) = F_{vdw}(1, s_{\text{Smin}} - s_o) \hspace{1cm} (3.23)$$
\[ F_{vdw}(1, s_{\text{min}}^R) \cdot s_{\text{min}}^R + \int_{s_{\text{min}}^R}^{s_{\text{max}}^R} F_{vdw}(1, s) ds = F_{vdw}(\theta, s_{\text{min}}^R) \cdot s_{\text{min}}^S + \int_{s_{\text{min}}^S}^{s_{\text{max}}^S} F_{vdw}(1, s - s_o) ds, \]

(3.24)

where \( \theta = (k_S/k_R)^{1/2} \) for Hookean contact model, and \( \theta = (Y_S/Y_R)^{2/5} \) for Hertzian contact model.

\( s_{\text{min}}^S \) and \( s_o \) can thus be obtained as solutions to Eqns. (3.23) and (3.24). It is noted that both values are independent from Hamaker constant as indicated by the equations. The values of \( s_{\text{min}}^S \) and \( s_o \) for spring stiffness employed in this study are calculated and summarized in Table 3.3.

Table 3.3: Model parameters for the modified van der Waals force model. Values are obtained by solving Eqns. (3.23) and (3.24).

<table>
<thead>
<tr>
<th></th>
<th>( k^S (N/m) )</th>
<th>( s_{\text{min}}^S (m) )</th>
<th>( s_o (m) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hookean contact model</td>
<td>100</td>
<td>( 1.384 \times 10^{-8} )</td>
<td>( 1.095 \times 10^{-8} )</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>( 4.777 \times 10^{-8} )</td>
<td>( 4.262 \times 10^{-8} )</td>
</tr>
<tr>
<td></td>
<td>( Y^S (Pa) )</td>
<td>( s_{\text{min}}^S (m) )</td>
<td>( s_o (m) )</td>
</tr>
<tr>
<td>Hertzian contact model</td>
<td>( 10^3 )</td>
<td>( 2.377 \times 10^{-8} )</td>
<td>( 2.007 \times 10^{-8} )</td>
</tr>
<tr>
<td></td>
<td>( 10^6 )</td>
<td>( 1.641 \times 10^{-7} )</td>
<td>( 1.548 \times 10^{-7} )</td>
</tr>
</tbody>
</table>

Using this new modified van der Waals force model, as shown in Figure 3.10(c), softer springs yield identical curves as the real spring. As shown in the figure, an analytical solution can be derived that describes this \( e_{\text{eff}} \) versus \( v_i \) curve. Assuming that the energy dissipated due to plastic deformation (viscous damping in the model) and cohesion are additive, it is found that

\[ e_{\text{eff}} = \sqrt{e_p^2 + e_c^2} - 1 \quad [130], \]

where \( e_c = \sqrt{1 - 2W_c/(mv_i^2)} \), and \( e_p \) is the elastic-plastic restitution coefficient (restitution coefficient for non-cohesive particles). The total work performed by cohesion \( W_c \) can be approximated by \( f_{v,ik}(A^R, s_{\text{min}}^R)l_c \). Thus, an analytical solution is derived:

\[ e_{\text{eff}} = \sqrt{e_p^2 - 2f_{v,ik}(A^R, s_{\text{min}}^R)l_c/(mv_i^2)}, \]

(3.25)
where $l_c$ is an adjustable parameter. For Figure 3.10 (c), $l_c = 1.25 \times 10^{-10}$ m is used. The excellent agreement between the analytical solution and the simulated results suggests the validity of this derivation.

It is found that these modifications can also be made to the expression $f_{v,iw}$ (Eqn. (3.12)) for van der Waals force between a particles and a flat surface. The modified model is following:

$$f_{v,iw}^M = -f_{v,iw}^M n_{iw} = \begin{cases} \frac{A_R r_p}{6(s-s_0)^2} n_{iw} & \text{for } s_{\text{min}}^S < s < s_{\text{max}} \equiv r_i/4 \\ -\frac{A_S r_p}{6s_{\text{min}}^S} n_{iw} & \text{for } s \leq s_{\text{min}}^S. \end{cases}$$

(3.26)

The values for $s_{\text{min}}^S$ and $s_o$ are found by solving Eqns. (3.23) and (3.24).

It was postulated in the above derivation that the potential energy $E_e$ at the maximum overlap distance is equal to the initial kinetic energy $E_k$. Strictly speaking, this is valid only for elastic and non-cohesive particles. For inelastic and/or cohesive particles, $\alpha = E_e/E_k$ depends on the value of the coefficient of restitution and the strength of cohesion. Allowing for $\alpha$ in the above derivation, and requiring that it be the same in the simulations with real and soft particle stiffness, for Hookean contact, we get $1/2k_R \delta_{\text{max}}^{R^2} = \alpha E_k = 1/2k_S \delta_{\text{max}}^{S^2}$, which leads to the same conclusion that $\delta_{\text{max}}^R/\delta_{\text{max}}^S = (k_S/k_R)^{1/2}$. For Hertzian contact, we get $Y_R \delta_{\text{max}}^{R5/2}/\alpha = Y_S \delta_{\text{max}}^{S5/2}/\alpha$, and thus $\delta_{\text{max}}^R/\delta_{\text{max}}^S = (Y_S/Y_R)^{2/5}$. This observation is confirmed by Figure 3.11, which demonstrates that this new modified van der Waals force model applies even when the restitution coefficient is lowered to 0.3 for both Hookean and Hertzian contacts.

The analysis above does not consider friction. To test whether the modified cohesion model also performs well for binary collision when friction is involved, extensive tests are performed for the following two cases: (1) head-on collision for particles with rotations (2) oblique collision for particles with rotations. Particle velocities after collision are compared, and it
Figure 3.11: Effective restitution coefficients versus impact velocities for various spring constants as per the legend for (a) Hookean contact and (b) Hertzian contact. The full modified van der Waals force model is used (Eqns (3.20)). Restitution coefficient $e$ of 0.3 is used. The curves represent the model predictions from Eqn. (3.25) with $l_c = 1.05 \times 10^{-9}$ m in (a) and $l_c = 1.12 \times 10^{-9}$ m in (b).

is found that the modified cohesion model yields results that are essentially independent of spring stiffness in these tests (details not shown).

Previous work by Kobayashi et al. [117] found that as their cohesion model was derived based on the analysis of a binary collision instead of aggregate collision, the model was not good for the case in which aggregates occupy a large fraction of the system. The cohesion models presented in this study (Eqn. (3.20)) are also based on binary collision analysis. Hence, it is likely to be deficient when one is fluidizing agglomerates. To assess this issue, we performed simulations of agglomerates as follows. To simplify the analysis, one dimensional velocities are considered. As shown in Figure 3.12, initially 16 stationary particles are positioned right next to each other. One particle on one end of the chain is given an initial velocity $v_i$ of 0.02 m/s in the direction towards the other particles, and simulations are run until the velocities of all the particles reach steady states.

The steady-state particle velocities are obtained and their distributions are plotted in Figure 3.13. Although not shown here, particles having the same velocities stay in one agglomer-
Figure 3.12: Configuration of the simulation on a collision between a particle and an agglom-erate. Particles are positioned right next to each other. In the beginning of the simulation, one particle in the end of the chain acquires a velocity $v_i$ of 0.02 m/s.

As shown in Figures 3.13(a)(b), as expected, soft spring constants using the original cohesion models yield very different particle velocities from the real spring constant. As shown in Figure 3.13(a), for $k = 100 N/m$, softer spring constant using the modified cohesion models yields similar particle velocity distribution as the real spring constant. However, as shown in Figure 3.13(b), for $k = 10 N/m$, even though softer spring constant using the modified cohesion model brings the particle velocity distribution closer to the real spring constant than using the original cohesion model, there are indeed some non-negligible differences. Specifically, the simulations with 7000 N/m yields only one particle having a negative velocity, whereas the simulation with 10 N/m using the modified cohesion model yields an agglomerate of two particles having negative velocities. Thus, for collisions involving large agglomerates, modified cohesion model might yield different results if a substantially softer spring (e.g. $k = 10 N/m$) is used, which is consistent with the finding by Kobayashi et al. [117].

As shown in the fluidization results later, this discrepancy would cause major changes to the flow patterns for the systems where dominant number of particles are in large agglomerates. (In other words, the modification to the van der Waals force model proposed here allows use of softer springs, but there is a limit on how soft one can make the spring.)

Cohesive particles with the modified cohesion model

Same analysis as described in subsections 3.1.4 and 3.1.4 is performed for particles with smaller spring constants using the modified cohesion models (Eqns. (3.20) and (3.26)). Group A particles ($A = 2.1 \times 10^{-21} J$) are studied first. Several snapshots at different times in the statistical steady state for Hookean contact model are shown in Figure 3.6 (rows 3 and 5
Figure 3.13: Distribution of steady-state particle velocities from the simulations for the collision between a particle and an agglomerate. Softer springs using both original and modified cohesion models are compared with the real spring for (a) $k = 100 \, N/m$ and (b) $k = 10 \, N/m$.

for $k$ of $100 \, N/m$, and $10 \, N/m$, respectively). As shown in the figure, using the modified cohesion models, similar flow behaviors to those with real spring constants are obtained for smaller spring constants. Specifically, similar sizes of the agglomerates are observed, and bubbles have similar shapes and sizes. The cumulative volume fraction of bubble diameter, shown in Figure 3.7(a) confirms that smaller spring constants with the modified cohesion models do yield similar bubble size distribution as those with realistic spring constants.

Same analysis on Group A particles is performed using Hertzian contact model and similar results are obtained. Representative snapshots at steady state are presented in Figure 3.8. Cumulative volume fraction of bubble diameters is included in Figure 3.4(b). For particles with smaller spring constants, when the modified cohesion model is used instead of the original cohesion model, similar sizes of agglomerates and bubble shapes are obtained as those with realistic spring constants. In addition, similar bubble size distribution is achieved.

Group C particles ($A = 4.2 \times 10^{-20} \, J$) are then considered for particles with smaller spring constants. Several snapshots at different time steps during initial fluidization period are
shown in Figure 3.9 (rows 3 and 5 for $k$ of 100 N/m, and 10 N/m, respectively). As shown in the figure, for $k = 100$ N/m with the modified cohesion model, similar flow behaviors are observed as those with $k = 7000$ N/m. A crack is initially formed at the bottom of the bed, and then travels up through the bed. However, for $k = 10$ N/m with the modified cohesion model, different flow behaviors are observed from those with $k = 7000$ N/m, as more than one crack is formed. As analyzed for the case of particle-agglomerate collision in subsection 3.1.4, for particles with substantially smaller spring constants (e.g. $k = 10$ N/m), the modified cohesion model would yield different results for collisions involving large agglomerates. For the fluidization of Group C particles here, almost all the particles are in large agglomerates. Thus, collisions between large agglomerates, rather than particles, are dominant in the system. As a result, different flow patterns are observed for $k = 10$ N/m, even when the modified cohesion model is used.

3.1.5 Conclusions

Gas-fluidization simulations with both Hookean and Hertzian contacts are performed. It is found that for non-cohesive particles, the flow patterns are insensitive to particle stiffness. However, for cohesive particles (Group A and Group C), the flow patterns are changed substantially when softer particles are used.

A theoretical analysis is then performed on two-particle collision, and a modified cohesion model is derived based on the analysis. The effective restitution coefficients strongly depend on particles stiffness when the original cohesion model is used. They become stiffness-independent with this modified cohesion model. For the particles with real particle stiffness ($k^R$ for Hookean contact model and $Y^R$ for Hertzian contact model), the original cohesion model can be used. The original cohesion models for particle-particle interaction ($f_{v,ik}$, illustrated by thick solid lines in Fig. 3.1) and particle-wall interaction ($f_{v,iw}$) are summarized.
as below:

\[
f_{v,ik} = -f_{v,ik} n_{ik} = \begin{cases} 
-F_{vdw}(A^R, s) n_{ik} & \text{for } s_{\text{min}}^R < s < s_{\text{max}}^R \equiv (r_i + r_j)/4 \\
-F_{vdw}(A^R, s_{\text{min}}) n_{ik} & \text{for } s \leq s_{\text{min}}^R
\end{cases}
\] (3.27)

\[
f_{v,iw} = -f_{v,iw} n_{iw} = \begin{cases} 
-A_{R_p}^s n_{iw} & \text{for } s_{\text{min}}^R < s < s_{\text{max}}^R \equiv r_i/4 \\
-A_{R_p}^s n_{iw} & \text{for } s \leq s_{\text{min}}^R
\end{cases}
\] (3.28)

where \(F_{vdw}(A, s)\) is defined in Eqn. (3.10).

For the softer particles (\(k^S\) for Hookean contact model and \(Y^S\) for Hertzian contact model), the modified cohesion models need to be used. The modified cohesion models for particle-particle interaction \(f_{v,ik}^M\) illustrated by thick dashed lines in Fig. 3.1) and particle-wall interaction \(f_{v,iw}^M\) are summarized as below:

\[
f_{v,ik}^M = -f_{v,ik}^M n_{ik} = \begin{cases} 
-F_{vdw}(A^R, s - s_o) n_{ik} & \text{for } s_{\text{min}}^S < s < s_{\text{max}}^S \equiv (r_i + r_j)/4 \\
-F_{vdw}(A^S, s_{\text{min}}^R) n_{ik} & \text{for } s \leq s_{\text{min}}^S
\end{cases}
\] (3.29)

\[
f_{v,iw}^M = -f_{v,iw}^M n_{iw} = \begin{cases} 
-A_{R_p}^s n_{iw} & \text{for } s_{\text{min}}^S < s < s_{\text{max}}^S \equiv r_i/4 \\
-A_{S_p} n_{iw} & \text{for } s \leq s_{\text{min}}^S
\end{cases}
\] (3.30)

Here, \(A^S\) is calculated by \(A^S = A^R(k^S/k^R)^{1/2}\) for Hookean contact model and \(A^S = A^R(Y^S/Y^R)^{2/5}\) for Hertzian contact model. \(s_o\) and \(s_{\text{min}}^S\) are additional model parameters, and can be found by solving the following equations:

\[
F_{vdw}(\theta, s_{\text{min}}^R) = F_{vdw}(1, s_{\text{min}}^S - s_o)
\] (3.31)
\[ F_{vdw}(1, s^R_{\text{min}}) \cdot s^R_{\text{min}} + \int_{s^R_{\text{min}}}^{s_{\text{max}}} F_{vdw}(1, s) ds = f_{v,ik}(\theta, s^R_{\text{min}}) \cdot s^S_{\text{min}} + \int_{s^S_{\text{min}}}^{s_{\text{max}}} F_{vdw}(1, s - s_o) ds, \]

(3.32)

where \( s_{\text{max}} = (r_i + r_j)/4 \). \( \theta \) is \((k_S/k_R)^{1/2}\) for Hookean contact model and \((Y_S/Y_R)^{2/5}\) for Hertzian contact model. Values of \( s_o \) and \( s^S_{\text{min}} \) for the particle stiffness in this study are included in Table 3.3.

This modified cohesion model is first tested for Group A particles. It is found that the flow behaviors become insensitive to particle stiffness. The modified cohesion model is then tested for Group C particles. It is found that if a substantially smaller particle stiffness is used, the flow behaviors are changed even with the modified cohesion model. The modified cohesion model is based on two-particle collision. As analyzed for particle-agglomerate collision, the modified cohesion model would yield different results when large agglomerates are involved in the collision. For Group C particles, collisions involving large agglomerates are dominant. These considerations introduce a limit to how soft one can make the contact model. Based on the results of this study, we could lower the spring constant by two orders of magnitude (from realistic values) with nearly similar results, but lowering it by three orders of magnitude led to unrealistic results. The high spring constant value used in the study is close to that of real materials encountered in most fluidization problems; the present study demonstrates that the modified cohesion model can be used to lower the spring constant by up to two orders of magnitude from actual values with only a small effect on the flow.
3.2 Investigation into the effects of fines on fluidization through CFD-DEM simulations

3.2.1 Introduction

It is well-known that size distribution of particles plays a crucial role on fluidization process. Many experimental studies [131–139] have shown that the addition of fines (typically defined as particles smaller than 45 µm) improves quality of fluidization, reduces bubble sizes, and increases reaction rates.

Beetstra et al. [139] investigated the effects of particle size distribution on the fluidization characteristics of Geldart Group A particles [9], and made the following observations: (1) The addition of fines reduces bubble sizes in fluidization of Group A particles; (2) Increasing amount of fines in the system results in greater bubble size reductions. However, the exact mechanism through which the addition of fines reduces the bubble sizes in the system is still under debate [139]. Several mechanisms have been discussed:

- Fines act as a kind of lubricant to lower the effective viscosity of the dense phase [140]. Specifically, it has been shown through experiments [140] that the effective viscosity of the dense phase in a fluidized bed of group A particles decreases with increasing fines contents. Lowered viscosity of the dense phase helps split the voids [141]. However, experiments by Beetstra et al. [139] found that when the binary mixture containing fines is compared to monodisperse particles with the same Sauter mean diameter, only a slight decrease of viscosity is observed, and is not significant enough to explain the decrease in the bubble size.

- It has been found from experiments [138, 142] that a broader particle size distribution results in a more expanded dense phase, which is consistent with the experiments [134]
which found that an increased bed expansion accompanies an increasing amount of fines during the start-up of fluidization. With the porosity of the dense phase increased, it leads to more interstitial gas passing through the dense phase at the expense of the bubble phase [133]. However, separate experiments by Khoe et al. [143] and Saayman et al. [131] both showed that the porosity of the dense phase is decreased with the addition of fines.

- It has been found from experiments [137] that a broader particle size distribution leads to more particles inside the dilute phase, which helps reduce the bubble size. This result is consistent with the collapse tests by Khoe et al [143], who reported that for a given average surface-volume diameter, a wide size distribution gives a greater air retention capacity than a bimodal distribution, which in turn gives greater retention than a narrow distribution. Also, Beetstra et al. [139] noticed that more solids rain through the bubbles in the case with fines. Grace and Sun [144] also provided theoretical considerations to rationalize that, not only more particles are present in the dilute phases when the particle size distribution is broadened, but also there is a disproportionate quantity of fines in the dilute phases compared with the particle size distribution in the bed as a whole. Specifically, some fines have terminal settling velocities of similar magnitude to the throughflow gas velocity inside the bubble, so that they can stay suspended in the voids as the voids travel for considerable distances.

A summary of these previous experimental investigations is also included in Table 3.4. Clearly, despite the universal agreement on the existence of bubble size reduction with addition of fines, previous experimental studies offer seemingly contradictory evidences on the exact mechanism through which fines reduce bubble sizes. It is suspected that the discrepancy might be due to the fact that particle properties and fluidization conditions are different for various experiments, which complicates the analysis by introducing other variables besides the addition of fines. Also, the addition of fines changes both cohesiveness and particle
Table 3.4: Summary of previous experimental investigations.

<table>
<thead>
<tr>
<th>Authors</th>
<th>Systems Studied</th>
<th>Findings</th>
</tr>
</thead>
<tbody>
<tr>
<td>Kono et al. [140]</td>
<td>Fluidization of FCC particles with fines.</td>
<td>Increasing fines contents lowers effective viscosity of the dense phase.</td>
</tr>
</tbody>
</table>
| Beetstra et al. [139] | Fluidization of alumina particles with PSD and fines.| (1) Only a slight decrease of viscosity with fines; not significant enough for decrease in bubble size.  
(2) More solids rain through the bubbles in the case with fines. |
| Kono et al. [142]     | Collapse experiments for FCC particles with fines.   | Fines increase dense phase porosity.                                    |
| van Ommen et al. [134]| Fluidization of alumina particles with fines.        | An increasing amount of fines leads to an increased bed expansion.       |
| Yates and Newton [133]| Fluidization of commercial oxidation catalyst with fines. | Fines increases dense phase porosity and allows more gas to pass through it. |
| Khoe et al. [143]     | Collapse experiments for FCC particles and glass beads with fines. | (1) Wider PSD decreases dense phase porosity.  
(2) Wider PSD gives a greater air retention capacity. |
| Saayman et al. [131]  | Fluidization of iron-silicon particles with fines.   | Fines decrease dense phase porosity.                                    |
| Sun and Grace [137]   | Fluidization of FCC particles with PSD.              | Wider PSD leads to more particles inside the dilute phase.              |
size distribution in the system, and in experiments it is exceedingly difficult to separate and pinpoint the effects from cohesiveness of particles and those from particle size distribution. Numerical simulations, on the other hand, can offer unique capabilities as one can untangle the effects from cohesion and particle size distribution. CFD-DEM approach is particularly attractive as it can easily account for particle size distribution and inter-particle cohesion. Indeed, CFD-DEM simulations have been successfully used to study fluidization with inter-particle cohesion [111–114, 117, 145] and particle size distributions [146]. However, there are no simulations specifically focusing on the effects of fines on bubble size reduction in fluidization. Here, we perform CFD-DEM simulations, and demonstrate that bubble size reduction with the addition of fines can indeed be captured by simulations. We identify the minimum physics required to observe such bubble size reductions, and propose a mechanism through which the addition of fines suppresses bubble formations.

### 3.2.2 Simulation conditions

In experimental studies on fluidization characteristics, particles are loaded into a tube equipped with a distributor and the superficial gas velocity is varied in a systematic manner to sample different expanded states. The dynamics observations in such experiments reflect a combination of bed and boundary effects. Typically, the beds by themselves are known to induce dynamic flow structures, even when walls are far away; the proximity of the bounding walls modifies this dynamics.

As detailed in Section 3.1.2, CFD-DEM simulations with the developed modified cohesion model are performed. CFD-DEM simulations of the type examined in the present study are expensive. Even a very small simulation domain (0.0052 m × 0.0052 m × 0.01014 m) requires tracking as many as 1.8 million particles. So, simulating fluidized beds of the kind used in experiments through this approach is infeasible. If one tries to include bounding walls in such small-domain simulations, the outcome would be dominated by wall effects and may not be
representative of bed-induced phenomena. For example, in such small-diameter pipes, the inhomogeneous flow would very quickly morph into slugging flow, while more realistically sized beds would manifest bubbling flow.

Simulations in periodic domains allows one to examine the bed dynamics without wall-induced restrictions, thus permitting isolation of dynamic characteristics that are attributable to bed. Such periodic domain simulations are widely employed in other problems such as Direct Numerical Simulation of isotropic turbulence. In the context of fluidized beds, analysis of dynamics in periodic domains [147–149] have exposed the hierarchy of inhomogeneities in fluidized beds that are entirely due only to the bed (and not the boundaries).

In the present study, we seek to examine if the effect of fines can be rationalized purely by their effect on bed dynamics (without requiring bounding walls). With this in mind, we perform simulations in periodic domains. The domain takes the form of a vertically oriented rectangular prism. For the Hertzian contact model, a soft Young’s modulus $Y_S$, instead of the real Young’s modulus $Y^R$, is used. As discussed in the previous section, to take account of this soft Young’s modulus, the modified cohesion model is used. The simulation parameters are provided in Table 3.5. Hamaker constants of typical metal oxide catalysts (such as alumina) [150, 151] are used.

At the beginning of a simulation, a fixed number of particles composed of base particles and various weight percent of fines are randomly put into the simulation box to achieve the desirable domain-averaged solid volume fraction $\langle \phi \rangle$.

To drive the flow in this periodic domain, we decompose the pressure term $p_g$ in Eqn. (3.14) into two components as follows: $p_g(\mathbf{x}, t) = p''_g(\mathbf{x}, t) - \bar{\rho}g(z - z_o)$. $p''_g$ is the computed gas pressure that obeys the periodic boundary condition. We add $-\bar{\rho}g(z - z_o)$ to drive the flow in the periodic domain. $\bar{\rho}$ is the domain-averaged mixture density. $z$ is the coordinate in the direction that is opposite of the gravity. $z_o$ is a reference coordinate. The simulations
Table 3.5: Parameter values used in the simulations.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Domain size; ((m \times m \times m))</td>
<td>(0.0052 \times 0.0052 \times 0.0104)</td>
</tr>
<tr>
<td>Acceleration due to gravity; (g) ((m/s^2))</td>
<td>9.81</td>
</tr>
<tr>
<td>Base particle diameter; (d_b^p) ((\mu m))</td>
<td>75</td>
</tr>
<tr>
<td>Fine particle diameter; (d_f^p) ((\mu m))</td>
<td>25</td>
</tr>
<tr>
<td>Particle density; (\rho_p) ((kg/m^3))</td>
<td>1500</td>
</tr>
<tr>
<td>Real Young’s modulus; (Y^R) ((Pa))</td>
<td>(7 \times 10^{10})</td>
</tr>
<tr>
<td>Soft Young’s modulus to be used in simulations; (Y^S) ((Pa))</td>
<td>10^8</td>
</tr>
<tr>
<td>Poisson’s ratio; (\nu)</td>
<td>0.42</td>
</tr>
<tr>
<td>Restitution coefficient; (e)</td>
<td>0.9</td>
</tr>
<tr>
<td>Sliding friction coefficient; (\mu_s)</td>
<td>0.5</td>
</tr>
<tr>
<td>Real Hamaker constant; (A^R) ((J))</td>
<td>(10^{-19})</td>
</tr>
<tr>
<td>Minimum separation distance for real Young’s modulus; (s_{R_{min}}^R) ((m))</td>
<td>(10^{-9})</td>
</tr>
<tr>
<td>Minimum separation distance for soft Young’s modulus; (s_{R_{min}}^S) ((m))</td>
<td>(2.377 \times 10^{-8})</td>
</tr>
<tr>
<td>Model parameter; (s_o)</td>
<td>(2.007 \times 10^{-8})</td>
</tr>
<tr>
<td>Gas density; (\rho_g) ((kg/m^3))</td>
<td>1.3</td>
</tr>
<tr>
<td>Gas viscosity; (\mu_g) ((Pa s))</td>
<td>(1.8 \times 10^{-5})</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Dimensionless/Characteristic Quantity</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fine particle diameter; (d_f^p) ((d_b^p))</td>
<td>1/3</td>
</tr>
<tr>
<td>Domain size; ((d_b^p \times d_b^p \times d_b^p))</td>
<td>(69 \times 69 \times 139)</td>
</tr>
<tr>
<td>Grid size; ((d_b^p \times d_b^p \times d_b^p))</td>
<td>(2 \times 2 \times 2)</td>
</tr>
<tr>
<td>Stokes relaxation time for base particle; (\tau_s^b) ((s))</td>
<td>0.026</td>
</tr>
<tr>
<td>Stokes relaxation time for fine particle; (\tau_s^f) ((s))</td>
<td>0.0029</td>
</tr>
<tr>
<td>Terminal velocity for a base particle ; (v_t^b) ((m/s))</td>
<td>0.2185</td>
</tr>
<tr>
<td>Terminal velocity for a fine particle ; (v_t^f) ((m/s))</td>
<td>0.0278</td>
</tr>
<tr>
<td>Froude number ; (Fr_t^b = \frac{v_t^b}{\sqrt{gd_b^p}})</td>
<td>64.9</td>
</tr>
<tr>
<td>Froude number ; (Fr_t^f = \frac{v_t^f}{\sqrt{gd_f^p}})</td>
<td>3.2</td>
</tr>
</tbody>
</table>

are run until the domain-averaged slip velocities \(\langle u_{slip} \rangle\) for both base and fine particles have achieved a sustained period of statistical steady state. \(\langle u_{slip} \rangle\) is defined as the difference between the Favre-averaged velocity of the gas and the average velocity of all the respective particles in the domain, and is scaled with terminal velocity for a base particle based on Wen and Yu [51] drag law \(v_t^b\). As illustrated in Figure 3.14 for the case of no cohesion and 3 wt% addition of fines, \(\langle u_{slip} \rangle/v_t^b\) for both particles reach steady state around \(t/\tau_s^b = 10\), where \(\tau_s^b\) is the Stokes relaxation time for base particles. \(\langle u_{slip} \rangle/v_t^b\) for both particles fluctuate as inhomogeneities are developed in the system. They fluctuate in the same way, indicating
that the system is well-mixed and no size segregation is present. \( \langle u_{\text{slip}} \rangle / v_t^b \) is always higher for base particles than for fine particles, which is expected as base particles require larger slip velocities to be fluidized. To characterize the bubble size, many snapshots of the system are taken at the steady state period (e.g. Figure 4.1). For each snapshot, the solid volume fraction values for all computational cells are converted to a binary image (return 1 for \( \phi < 0.15 \) and 0 for \( \phi > 0.15 \)). A different cutoff solid volume fraction of 0.05 instead of 0.15 is also considered, and similar results are obtained. Specifically, Figure 3.20 is repeated using the cutoff solid volume fraction value of 0.05 instead of 0.15. As shown in the Figure 3.15, this reduction slightly decreases the size of the bubbles. The addition of fines suppressing bubble formation at high solid volume fraction is still observed. Thus, the choice of the minimum does not affect the conclusions drawn in this study. The built-in function called bwconncomp in MATLAB® Image Processing Toolbox [152] employing a flood-fill algorithm with connectivity of 26 is then used to find connected cells. Clusters of connected cells are identified and the bubble volume \( V_b \) can be computed by multiplying the number of cells in each cluster with the cell volume. Bubble volumes are collected from all the snapshots, and the effective bubble diameter for each bubble volume \( d_{\text{bubble}} \) is given by \( (6V_b/\pi)^{1/3} \).
Figure 3.15: Volume medium scaled bubble diameter \( \bar{d}_{\text{bubble,}50} \) versus domain-averaged solid volume fraction \( \langle \phi \rangle \). The cutoff solid volume fraction of 0.05 is used. Cohesion is included. The results are presented for different levels of fines added to base particles as per the legend. The lower and upper limits of the error bars represent \( \bar{d}_{\text{bubble,}40} \) and \( \bar{d}_{\text{bubble,}60} \), respectively. Similar results are obtained here as in Figure 3.20 where the cutoff value of 0.15 is used instead.

The effective bubble diameter is scaled with base particle diameter \( d_p \) to yield \( \bar{d}_{\text{bubble}} \). As an illustrative example, the cumulative volume fraction of bubbles are plotted against the scaled bubble diameter, as shown in Figure 3.17 for the case of non-cohesive particles without fines at \( \langle \phi \rangle = 0.45 \). As indicated in the figure, the volume medium scaled bubble diameter, \( \bar{d}_{\text{bubble,}50} \), is then identified. 50\% of total bubble volume is comprised of bubbles whose \( \bar{d}_{\text{bubble}} \) are smaller than \( \bar{d}_{\text{bubble,}50} \). Similarly, \( \bar{d}_{\text{bubble,}40} \) and \( \bar{d}_{\text{bubble,}60} \) are calculated, which correspond to the cases where 40\% and 60\% of total bubble volume are comprised of bubbles whose \( \bar{d}_{\text{bubble}} \) are smaller than \( \bar{d}_{\text{bubble,}40} \) and \( \bar{d}_{\text{bubble,}60} \), respectively.

The macroscopic stress tensor is calculated as \( \sigma = \frac{1}{V} \sum_i \left[ \sum_{j \neq i} \frac{1}{2} \mathbf{r}_{ij} \mathbf{f}_{ij} + m_i (\mathbf{v}_i') (\mathbf{v}_i') \right] \), where \( V \) is the total volume of the domain, \( \mathbf{r}_{ij} \) is the normal vector pointing from the center of particle \( j \) to that of particle \( i \), \( \mathbf{f}_{ij} \) is the total force experienced by particle \( i \) from particle \( j \), and \( \mathbf{v}_i' \) is the fluctuating velocity of particle \( i \) relative to the domain-averaged particle velocity. This stress tensor is further ensemble-averaged over many time steps during the steady state.
Figure 3.16: Snapshots of the fluidized systems colored with local solid volume fraction for different cases. In (a), no cohesion or fines is present. In (b), no cohesion is present, and 3 wt% fines are added. In (c), cohesion is present, and 3 wt% fines are added. The domain-averaged solid volume fraction $\langle \phi \rangle$ is 0.45 for all the cases. Bubbles with comparable sizes are readily identified in (a) and (b). No bubbles are observable in (c).

Figure 3.17: Cumulative volume fraction of bubbles collected from the snapshots versus the respective $d_{\text{bubble}}$. The domain-averaged solid volume fraction $\langle \phi \rangle$ is 0.45. No fines are added, and cohesion is not included. Here, the bubble size is made dimensionless using the base particle diameter.
Ensemble-averaged pressure $p$ is calculated as $p = (\sigma_{xx} + \sigma_{yy} + \sigma_{zz})/3$. To characterize the microstructure of the system, the average coordination number for all particles ($Z$) and the average coordination number for base particles ($Z_b$) are computed. $Z$ is the average number of contacts per particle in the system, and computed as $Z = 2n_c/n$, where $n_c$ is the total number of contacts (with particle overlap) and $n$ is the total number of particles in the system. $Z_b$ is the averaged number of contacts experienced by the base particle per base particle in the system, and computed as $Z_b = (2n_{bb}^b + n_{bf}^b)/n_b$, where $n_{bb}^b$ is the total number of contacts between two base particles, $n_{bs}^b$ is the total number of contacts between a base particle and a fine particle, and $n_b$ is the total number of base particles in the system. Both $Z$ and $Z_b$ are also ensemble-averaged over many time steps during the steady state.

### 3.2.3 Results and discussions

**The effects of fines on bubble sizes without cohesion**

We first perform simulations without taking account of the interparticle van der Waals forces. The results on $d_{\text{bubble},50}$ at different domain-averaged solid volume fractions for different amount of fines added to the system are presented in Figure 3.18. The figure shows that the bubble size is essentially insensitive to the addition of fines for $\langle \phi \rangle < 0.55$, and the size is increased with the addition of fines for $\langle \phi \rangle = 0.55$. For visual representations of the system at $\langle \phi \rangle < 0.55$, Figures 4.1 (a) and (b) present snapshots of the fluidized systems at $\langle \phi \rangle = 0.45$ colored with local volume fractions. For both cases, cohesion is not included. No fines are present in (a), while 3 wt% fines are added in (b). Bubbles with comparable sizes are visible for both cases. For $\langle \phi \rangle = 0.55$, it is found that the addition of fines increases the bubble sizes. A closer look at the cumulative volume fraction of bubbles at $\langle \phi \rangle = 0.55$ for various fines contents (Figure 3.19) further confirms this observation. As discussed before, experimentally it is found that the addition of fines reduces the size of bubbles.
Figure 3.18: Volume medium scaled bubble diameter $\overline{d}_{\text{bubble},50}$ versus domain-averaged solid volume fraction $\langle \phi \rangle$. Cohesion is not included. The results are presented for different levels of fines added to base particles as per the legend. The lower and upper limits of the error bars represent $\overline{d}_{\text{bubble},40}$ and $\overline{d}_{\text{bubble},60}$, respectively.

However, the simulations here show that the bubble size is insensitive to (for cases of $\langle \phi \rangle < 0.55$) or increased with (for cases of $\langle \phi \rangle = 0.55$) the addition of fines, which is contrary to the experimental observations. Furthermore, in the simulation results here, significantly large bubbles are present at high solid volume fractions. Experimentally, homogeneous non-bubbling bed expansion is observed during fluidization of Group A particles [9]. Thus, the simulation results here for the cases of no fines at high solid volume fractions are inconsistent with the fluidization behaviors of Group A particles. Both these observations suggest that simulations without accounting for the interparticle van der Waals forces yield results that are inconsistent with experimental observations.

**The effects of fines on bubble sizes with cohesion**

We then perform the same simulations, but now accounting for the interparticle van der Waals forces. The results on $\overline{d}_{\text{bubble},50}$ at different domain-averaged solid volume fractions for different amount of fines added to the system are presented in Figure 3.20. When no fines are present, for sufficiently high $\langle \phi \rangle$ ($\langle \phi \rangle \geq 0.5$), the bubbles are suppressed. These results are
Figure 3.19: Cumulative volume fraction of bubbles collected from the snapshots versus the respective $d_{\text{bubble}}$ for various fines contents. The domain-averaged solid volume fraction $\langle \phi \rangle$ is 0.55. Cohesion is not included. Here, the bubble size is made dimensionless using the base particle diameter.

consistent with the fact that Group A particles undergo a bubbleless uniform bed expansion during fluidization [9]. With the addition of fines, the bubbles can be suppressed at lower $\langle \phi \rangle$. When 3 wt% fines are added, the bubbles are suppressed at $\langle \phi \rangle$ as low as 0.45. Figure 4.1(c) illustrates such bubble suppression for $\langle \phi \rangle = 0.45$ with 3 wt% fines. The simulation results are consistent with previous experimental findings that the addition of fines increases the interval of homogeneous fluidization [134, 153]. When more fines are added, the bubbles can be suppressed at even lower $\langle \phi \rangle$. When 10 wt% fines are added, the bubbles are suppressed at $\langle \phi \rangle$ as low as 0.415. It is consistent with the experimental findings [139, 154] that increasing amount fines in the system are found to further reduce bubble size in the fluidized system. As discussed before, to characterize bubble sizes, a cutoff solid volume fraction of 0.15 is used in Figure 3.20. As shown in the Appendix, similar results are obtained when 0.05 is used instead of 0.15.

It should be noted that the exact critical volume fraction at which the transition from bubbling to homogeneous flow occurs depends the actual values of parameters employed. We focus on direction effects that this critical volume fraction decreases as fines content is increased. This decrease in the critical volume fraction with increasing fines can be compared
with the experiments, such as the one by Kono et al. [142]. In the experiments, Aluminum hydrate (particle diameter $13\mu m$) or Limestone (particle diameter $13\mu m$) are added as fines to FCC particles (particle diameter $70\mu m$), and the solid volume fractions at the minimum bubbling conditions ($\phi_{mb}$) are found through collapse experiments. In the simulations, $\phi_{mb}$ correspond to critical volume fraction at which the transition from bubbling to homogeneous flow occurs. $\phi_{mb}$ is compared between experiments and simulations for various fines contents as shown in Figure 3.21. As shown in the figure, increasing fines decrease $\phi_{mb}$ in a similar fashion between experiments and simulations. $\phi_{mb}$ is consistently higher for simulations than experiments, as the particles in the experiments are smaller and might be more cohesive than the ones specified in the simulations.

Due to the large number of particles introduced with the addition of fines, a relatively small simulation domain is studied here. To demonstrate that similar results can also be observed in larger domains, we perform additional simulations where the domain is increased by half for both width and depth. As shown in Figure 3.22, larger bubbles are observed in the increased domain. However, similar to the original domain, the bubbles in the larger domain are also suppressed for sufficiently high $\langle \phi \rangle$ ($\langle \phi \rangle \geq 0.5$). Furthermore, the bubble size reduction with the addition of fines is also observed in the larger domain. As shown in Figure 3.23, when accounting for cohesion, the addition of 3 wt% of fines suppresses the bubble formation at $\langle \phi \rangle = 0.45$. This behavior is consistent with the observation in the original domain (Figures 4.1(a)(c)). The bubble sizes observed in the simulations are rather small compared with those seen in the experiments, as they are limited by the domain sizes. As indicated by the simulation results here, as domain sizes become larger, the bubble sizes would also increase. However, the reductions of bubble sizes with the addition of fines would still be observed, as large bubbles arise in fluidized beds through bubble growth. When formation of smaller bubbles is suppressed, then the pathway to larger bubbles gets arrested. Consequently, one can learn about mechanisms that suppress bubbles at small scale by studying small test problems such as those studied here.
Figure 3.20: Volume medium scaled bubble diameter $\bar{d}_{\text{bubble},50}$ versus domain-averaged solid volume fraction $\langle \phi \rangle$. Cohesion is included. The results are presented for different levels of fines added to base particles as per the legend. The lower and upper limits of the error bars represent $\bar{d}_{\text{bubble},40}$ and $\bar{d}_{\text{bubble},60}$, respectively.

Figure 3.21: Solid volume fraction at the minimum bubbling condition ($\phi_{mb}$) for various fines contents found in experiments [142] and present simulations.
Figure 3.22: Volume medium scaled bubble diameter $\bar{d}_{\text{bubble},50}$ versus domain-averaged solid volume fraction $\langle \phi \rangle$. Cohesion is included. The results are presented for two different domain sizes, as per the legend. The original domain size is described in Table 3.5. The increased domain size doubles the width and depth. The lower and upper limits of the error bars represent $\bar{d}_{\text{bubble},40}$ and $\bar{d}_{\text{bubble},60}$, respectively.

Figure 3.23: Snapshots of the fluidized systems of an increased domain size colored with local solid volume fraction for different cases. In (a), no fines are added. In (b), 3 wt% fines are added. The domain-averaged solid volume fraction $\langle \phi \rangle$ is 0.45 for all the cases. The increased domain size doubles the width and depth of the original system described in Table 3.5. Bubbles are readily identified in (a), but no bubbles are observed in (b). Cohesion is included.
Figure 3.24: Scaled particle phase pressure $p_p/(d_p \rho g)$ versus domain-averaged solid volume fraction $(\phi)$. The van der Waals forces are included. The results are presented for different levels of fines added to base particles as per the legend.

**Stable solid-like regime**

Previous experiments [155] have been performed to study this characteristic expanded bed regime for Group A particles where bubbles are suppressed. It is found that at this regime, the particles are in a completely static state. Essentially all particles in the system are held by enduring contacts, and the stresses are carried by particle contacts instead of collisions. This stable solid-like regime is also observed in previous simulations [111] on fluidization behaviors of Group A particle at the expanded bed regime. It is found that the van der Waals forces are balanced with the contact forces, and the gravity force is balanced with the particle-fluid interaction force [111]. As a result, the particles have minimal velocity fluctuations in this regime. The average coordination number $Z$ is found to be increased, and provides mechanical stabilities against the upward gas flow. This increase in $Z$ and the emergence of this solid-like behavior with cohesion is also observed in the simple shear simulations of dense granular materials [156]. It is found that for solid volume fractions below the jamming volume fractions, the inclusion of cohesion would allow stress to become shear rate independent accompanied with an increase in average coordination number.
Figure 3.25: (a) Average coordination number for all particles $Z$ and (b) average coordination number for base particles $Z_b$, versus domain-averaged solid volume fraction $\langle \phi \rangle$. The van der Waals forces are included. The results are presented for different levels of fines added to base particles as per the legend.

We also observe the stable solid-like regimes in our results for the cases both with and without fines at sufficiently high $\langle \phi \rangle$. Specifically, as shown in Figure 3.24, the scaled particle phase pressure is essentially zero for all the cases with bubble size reduction (Figure 3.20). The particle phase pressure includes contributions from interparticle forces and particle velocity fluctuations. At the stable solid-like regime, the forces on each particle are balanced and particle velocity fluctuations are damped, which results in the particle pressure essentially zero. As shown in Figure 3.25, even though the average coordination number for all particles $Z$ does not increase significantly with the addition of fines, the average coordination number for base particles $Z_b$ increases substantially. This increase in $Z_b$ provides mechanical stabilities for base particles against the gas flow, and helps suppress bubble formation.

Both previous [111, 155, 156] and present studies indicate that interparticle cohesion is responsible for the formation of this stable solid-like regime. However, for the cases with the addition of fines, interparticle cohesion is present between two base particles, between two fine particles, as well as between one base particle and one fine particle. To pinpoint the cohesion that is essential for the formation of the stable solid-like regime, we probe further
the default case with 3 \textit{wt\%} fines and cohesion of all pairs at \(\phi = 0.45\) (Case 1 in Table 3.6).

As shown in Case 2 in Table 3.6, when only the base-base cohesion is turned off, the bubble sizes are not reduced. It indicates that the base-base cohesion is important for bubble size reduction. In Case 3, only base-fine cohesion is turned off, and the bubble sizes are not reduced. It indicates that the base-fine cohesion is also important for bubble size reduction.

In Case 4, only fine-fine cohesion is turned off, and the bubble sizes are still reduced. It indicates that fine-fine cohesion is not essential for bubble size reduction. When 12 \textit{wt\%} fines are added, the bubble sizes are still reduced when only base-base cohesion is turned off and when only fine-fine cohesion is turned off. In contrast, when base-fine cohesion is turned off, the bubble sizes are not reduced. Also, bubble sizes are not reduced if both base-base cohesion and fine-fine cohesion are not included. These results suggest that for 12 \textit{wt\%} fines, base-fine cohesion together with either base-base cohesion or fine-fine cohesion is needed for bubble size reduction. In conclusion, base-fine cohesion is essential for the stable solid-like regime. In addition, base-base cohesion (for both low and high fines content) or fine-fine cohesion (for high fines content) is needed to observe a bubble size reduction.

Table 3.6: Effects of interparticle cohesion pairs on bubble size reductions.

<table>
<thead>
<tr>
<th>Case</th>
<th>Base-Base</th>
<th>Base-Fine</th>
<th>Fine-Fine</th>
<th>Bubble Sizes</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Reduced</td>
</tr>
<tr>
<td>2</td>
<td>No</td>
<td>Yes</td>
<td>Yes</td>
<td>Not Reduced</td>
</tr>
<tr>
<td>3</td>
<td>Yes</td>
<td>No</td>
<td>Yes</td>
<td>Not Reduced</td>
</tr>
<tr>
<td>4</td>
<td>Yes</td>
<td>Yes</td>
<td>No</td>
<td>Reduced</td>
</tr>
<tr>
<td>5</td>
<td>No</td>
<td>Yes</td>
<td>Yes</td>
<td>Reduced</td>
</tr>
<tr>
<td>6</td>
<td>Yes</td>
<td>Yes</td>
<td>No</td>
<td>Reduced</td>
</tr>
<tr>
<td>7</td>
<td>Yes</td>
<td>No</td>
<td>Yes</td>
<td>Not Reduced</td>
</tr>
<tr>
<td>8</td>
<td>No</td>
<td>Yes</td>
<td>No</td>
<td>Not Reduced</td>
</tr>
</tbody>
</table>
Two-particle collision with cohesion

The formation of this stable solid-like regime from cohesion can be reasoned by considering two-particle collisions. As detailed in Simulation Methodology section, we simulate two particles with equal but opposite impact velocities undergoing a head-on collision, and calculate the corresponding effective restitution coefficients, for various impact velocity values. Here, the simulations are performed for collisions between two base particles, between two fine particles, and between one base particle and one fine particle. The effective restitution coefficients are plotted against the impact velocities in Figure 3.26. The particle properties used in the simulations are the same as those that are used before (Table 3.5). The shape of the curve is consistent with the experimental observations [128, 129]. In the experiments, microsized particles with different velocities normal to the surface impact with a flat surface, and the incoming and rebounding particle velocities are measured to calculate the corresponding restitution coefficient. In both the experiments and simulations here, there is a critical velocity $v_c$, below which the particles would not bounce back and stick to the flat surface or each other. For impact velocities larger but close to $v_c$, the effective restitution coefficient has a steep increase as the impact velocity increases. As the impact velocity further increases, the effective restitution coefficient increases slowly and eventually reaches an asymptote, which equals to the one for non-cohesive particle collision. It is this velocity dependent behavior of the effective restitution coefficient presented here which results from interparticle cohesion that causes the formation of the stable solid like regime observed for cases with and without fines. In both the experiments [128] and the simulations here, the critical velocity $v_c$ increases as the colliding particle diameter decreases. In the simulation results here, the critical velocity for collision between two base particles is $7 \times 10^{-4} \text{ m/s}$. It increases to $1.9 \times 10^{-3} \text{ m/s}$ for the collision between a base particle and a fine particle, and $2.1 \times 10^{-3} \text{ m/s}$ for the collision between two fine particles. Introducing fines into the systems allow base particles to collide with fine particles. As $v_c$ is higher between a base
Figure 3.26: Effective restitution coefficient versus impact velocity. Simulations are performed to model two particles with equal but opposite impact velocities undergoing a head-on collision, and the corresponding restitution coefficient is calculated. This collision is performed for various impact velocities for the collisions between two base particles, between a base particle and a fine particle, and between two fine particles, as per the legend. The simulation parameters are in Table 3.5. The modified cohesion model is used.

particle and a fine particle than between two base particles, particle fluctuation velocities can be dampened more frequently. As a result, the stable solid-like regime can form more easily. Increasing amount of fines in the system allows even more fine particles to collide with base particles, and dampen the velocity fluctuations. The importance of base-fine interaction discussed here is consistent with the previous subsection which concludes that base-fine cohesion is essential for bubble size reduction.

3.2.4 Conclusions

CFD-DEM simulations have been performed in a periodic box with fixed domain-averaged solid volume fraction ($\phi$) to investigate the effects of fines on bubble size reduction in fluidization of Group A particles. It is found that without cohesion, addition of fines does not reduce bubble sizes. Thus, particle size distribution alone cannot explain bubble size reduction due to addition of fines. With cohesion included, bubbles are suppressed at sufficiently high ($\phi$), corresponding to the expanded bed regime for Group A particles. With the addition of fines,
the bubbles can be suppressed at lower $\langle \phi \rangle$. With the addition of more fines, the bubbles can be suppressed at even lower $\langle \phi \rangle$. When bubbles are suppressed, the system is in a stable solid-like regime. In this regime, forces on each particle are balanced and particle velocity fluctuations are suppressed, resulting particle phase pressure approaching zero. The average coordination number for base particles is increased, and thus provides a mechanical stability for base particles against the upward gas flow. The cohesion between base and fine particles is found essential for the formation of this regime, as velocity fluctuation of base particles are dampened from the base-fine cohesion via their collisions with fine particles.

Thus, the work here is in agreement with the mechanisms through which fines reduce bubble sizes reported by previous experimental works [133, 134, 138, 142]. Specifically, the addition of fines results in a more expanded dense phase, and allows more interstitial gas to pass through at the expense of the bubble phase. Unlike these experiments, the current simulation work demonstrates that a more expanded dense phase is a direct result of the increased cohesion introduced by fines.
Chapter 4

Rheology of non-cohesive and cohesive granular materials in gas-fluidized suspensions

Overview of the chapter

We perform CFD-DEM simulations for gas-fluidization of frictional particles with and without interparticle van der Waals force in a fully periodic domain. By analyzing snapshots gathered from the simulations, quantities of interest in formulating a rheological model are determined. Unlike the studies in Chapter 2 through DEM-only simulations, this approach allows for taking account of the effects of interstitial fluid and covers a wider range of parameter space. We first validate this methodology using non-cohesive particles, and show that results obtained are consistent with the analytically derived kinetic theory in literature. Then, we analyze the results from cohesive particles. For dense flow regime, it is found that

\[1\] The work in this chapter is based a manuscript which has been submitted for journal publication: Y. Gu, A. Ozel, J. Kolehmainen, and S. Sundaresan. Computationally generated constitutive models for particle phase rheology in gas-fluidized suspensions.
both pressure and shear stress results are consistent with the ones from Chapter 2, thus further affirming the viability of the approach. For dilute flow regime, it is found that pressure follows a behavior similar to van der Waals equation of state. Specifically, at low granular temperatures, pressure from cohesion decreases with increasing solid volume fraction for a range of solid volume fractions. For particle shear stress, it is found that for a given solid volume fraction and increasing granular temperature, the shear stress initially decreases before increasing. This non-monotonic behavior is a result of the interplay between the cohesive energy and kinetic energy from particle agitation, which is found to be captured by a model based on the previously proposed fluidity approach.

4.1 Introduction

Eulerian models for gas-particle flows require as input a constitutive model for the particle phase stress. A great deal of work has been done in the literature on deriving constitutive models by adapting the kinetic theory of dense gases to particulate flows. The earliest and most widely used kinetic theory models have been derived for dilute flows of inelastic, smooth, frictionless spheres with no effects from interstitial fluid [18, 24–27]. They have been extended or modified to account for particle roughness [28, 157–159], dense regime [28, 29], decoupling of particle fluctuations into correlated and uncorrelated parts [160, 161], role of the interstitial fluid [18, 162–168], and cohesion [169–174].

An alternative way to simulate granular flows is through the discrete element method (DEM) [53]. Its strength lies in its flexibility to directly include particle size distribution [17, 60] (also see Chapters 2 and 3), complex particle-particle interactions including van der Waals forces [58], electrostatic forces [175], capillary forces [75], liquid bridges [176], solid bridges [76], the interstitial fluid through CFD-DEM [14], or a combination thereof (such as the study on fines in Chapter 3). However, such a method becomes impractical
for large number of particles, and consequently there has been efforts to deduce continuum rheological models based on DEM simulations [58, 63, 67, 69–71, 90, 108] (also in Chapter 2). Most of these simulations used to deduce models are based on particle-only DEM simulations where particles are sheared or flow down a slope. The deficiencies of these resultant models when applied to fluid-solid flows are threefold. First, the effects of interstitial fluid are not accounted for in these DEM simulations. Second, these simulations are mostly one-dimensional in nature, and thus the effects of dilation and compaction of the particle phase are not probed adequately. Third, it has been reported in several studies [177, 178] and Chapter 2 that local complex flow structures would form when cohesive forces are included in these simulations, whose effects are not fully captured by nearly one-dimensional flows.

These can be addressed through CFD-DEM simulations. CFD-DEM simulations have been used to deduce models for systems such as dilute gas-solid turbulent flows [179–182] and granular flows in bedload transport [183]. In the present study, we seek to deduce a rheological model for granular materials in fluidized suspensions from CFD-DEM simulations. First, we consider the case of non-cohesive particles fluidized by gas (section 4.3.1), and demonstrate that the approach yields models that are consistent with the analytically derived kinetic theory models, which indicates the validity of the methodology. We also show intriguing results that are previously not observed through traditional methods, such as the path-dependence of bulk viscosity and gravity-dependence of stress. Then, we demonstrate that this methodology can be used to cases where complex inter-particle interaction is important (section 4.3.2). We use the van der Waals force as an example, which is known to affect flow behaviors of Geldart Group A particles [9] that are frequently encountered in industries. We show that this approach yields results that are consistent with previous studies of cohesive particles [58] and the results in Chapter 2, thus further corroborating the methodology. Different from these studies, the present methodology is able to probe a wider parameter space. We then propose an ad hoc adaptation of the kinetic-theory-based model for granular
flows in the presence of van der Waals interaction between particles. This methodology can be readily applied to systems where other complex inter-particle interactions are present.

### 4.2 Simulation conditions

As detailed in Section 3.1.2, CFD-DEM simulations with the developed modified cohesion model are performed. We perform simulations in periodic domains in which one can examine the flow dynamics without wall-induced restrictions. To drive the flow in this periodic domain, we decompose the pressure term \( p_g \) in Eq. (3.14) into two components as follows:

\[
p_g(x, t) = p'_g(x, t) - \bar{\rho}|\mathbf{g}|(z - z_o).
\]

Here, \( p'_g \) is the computed gas pressure that obeys the periodic boundary condition and \( \bar{\rho}|\mathbf{g}|(z - z_o) \) represents the mean vertical pressure drop due to the total mass of a two-phase mixture; \( \bar{\rho} \) is the domain-averaged mixture density; \( z \) is the coordinate in the direction that is opposite of gravity and \( z_o \) is a reference elevation.

Although we will present our results in dimensionless form, it is useful to present typical dimensional quantities to demonstrate that the simulations have been done for gas-particle systems of practical interest. With this in mind, in table 4.1, we present the simulation parameters in both dimensional and dimensionless form. Simulations were performed for two domain-averaged solid volume fractions \( \langle \phi \rangle = 0.1 \) and 0.3 with different values of particle diameter and acceleration due to gravity (which was lowered to help probe relevant dimensionless groups). The simulations were run for a sufficiently long duration \( (10 \tau_{St}^p) \) to ensure that a statistical steady state is reached (see table 4.1 for the definition of \( \tau_{St}^p \)). Subsequently, snapshots were collected at every \( \tau_{St}^p \) time instant for a duration of \( 20 \tau_{St}^p \). Snapshots of the particle volume fraction fields obtained in simulations with different domain-averaged solid volume fractions for non-cohesive particles with \( Fr_p = 65 \) are shown in figure 4.1. The computational data from these snapshots were then post-processed to compute the particle
phase stress $\sigma$ and granular temperature $T$ for each cell with volume of $V_c$:

$$\sigma = \frac{1}{V_c} \sum_{i\in\text{cell}} \left[ \sum_{j\in\text{cell},(j\neq i)} \frac{1}{2} \mathbf{r}_{ij} \otimes \mathbf{f}_{ij} + m_i (\mathbf{v}_i - \mathbf{u}_{s|x=x_i}) \otimes (\mathbf{v}_i - \mathbf{u}_{s|x=x_i}) \right], \quad (4.1)$$

and

$$T = \frac{1}{3} \sum_{i\in\text{cell}} \left[ (\mathbf{v}_i - \mathbf{u}_{s|x=x_i}) \cdot (\mathbf{v}_i - \mathbf{u}_{s|x=x_i}) \right], \quad (4.2)$$

where $\mathbf{r}_{ij}$ is the unit vector pointing from the center of particle $j$ to that of particle $i$, $\mathbf{f}_{ij}$ is the total force between the two particles, $\mathbf{v}_i$ is the velocity of particle $i$, and $\mathbf{u}_{s|x=x_i}$ is the local-average particle velocity at the location of the particle, obtained by interpolating from the Eulerian velocity of the solid phase at the cell centers.

### 4.3 Simulation results

In fluidization, the normal stress in the vertical direction is usually larger than those in the lateral directions [166]. Normal stress differences were probed briefly in this study. Figure 4.2 plots scaled normal stress components $\frac{\sigma_i}{(1/3)\text{tr}(\sigma)}$ against solid volume fraction $\phi$. The data are from fluidization simulations of non-cohesive particles with $Fr_p = 65$. Horizontal normal stress components $\sigma_{xx}$ and $\sigma_{yy}$ are indistinguishable, to within computational accuracy. At higher volume fractions, the variation of stress is under $\pm 20\%$. As volume fraction decreases, the anisotropy increases. This behavior is expected as there are fewer collisions at lower volume fractions. As normal stress difference has not been demonstrated to be responsible for any known flow phenomena in fluidized beds, we have not probed them further in this study.
### Simulation Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Domain size; $(d \times d \times d)$</td>
<td>$240 \times 240 \times 960$</td>
</tr>
<tr>
<td>Grid size; $(d \times d \times d)$</td>
<td>$3 \times 3 \times 3$</td>
</tr>
<tr>
<td>Acceleration due to gravity; $g$ [m/s$^2$]</td>
<td>$9.81/2.45$</td>
</tr>
<tr>
<td>Particle diameter; $d$ [$\mu$m]</td>
<td>$75/150/300$</td>
</tr>
<tr>
<td>Particle density; $\rho_p$ [kg/m$^3$]</td>
<td>$1500$</td>
</tr>
<tr>
<td>Real Young’s modulus; $Y_R$ [Pa]</td>
<td>$7 \times 10^{10}$</td>
</tr>
<tr>
<td>Soft Young’s modulus used in simulations; $Y_S$ [Pa]</td>
<td>$10^6$</td>
</tr>
<tr>
<td>Poisson’s ratio; $\nu$</td>
<td>$0.42$</td>
</tr>
<tr>
<td>Restitution coefficient; $e_p$</td>
<td>$0.9$</td>
</tr>
<tr>
<td>Sliding friction coefficient; $\mu_p$</td>
<td>$0.5$</td>
</tr>
<tr>
<td>Real Hamaker constant; $A^R$ [J]</td>
<td>$10^{-19}/10^{-18}$</td>
</tr>
<tr>
<td>Minimum separation for real Young’s modulus; $s_{\text{min}}^R$ [m]</td>
<td>$10^{-9}$</td>
</tr>
<tr>
<td>Minimum separation for soft Young’s modulus; $s_{\text{min}}^S$ [m]</td>
<td>$1.641 \times 10^{-7}$</td>
</tr>
<tr>
<td>Modified cohesion model parameter; $s_o$ [m]</td>
<td>$1.548 \times 10^{-7}$</td>
</tr>
<tr>
<td>Gas density; $\rho_g$ [kg/m$^3$]</td>
<td>$1.3$</td>
</tr>
<tr>
<td>Gas viscosity; $\mu_g$ [Pa s]</td>
<td>$1.8 \times 10^{-5}$</td>
</tr>
</tbody>
</table>

### Characteristic Quantities

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stokes relaxation time; $\tau_{p}^{St} = \frac{\rho_p d^2}{18 \mu_g}$ [s]</td>
<td>$0.026$ ($d = 75 \mu$m)</td>
</tr>
<tr>
<td></td>
<td>$0.104$ ($d = 150 \mu$m)</td>
</tr>
<tr>
<td></td>
<td>$0.417$ ($d = 300 \mu$m)</td>
</tr>
<tr>
<td>Terminal velocity based on Wen and Yu drag law; $v_t$ [m/s]</td>
<td>$0.219$ ($d = 75 \mu$m; $g = 9.81$ m/s$^2$)</td>
</tr>
<tr>
<td></td>
<td>$0.649$ ($d = 150 \mu$m; $g = 9.81$ m/s$^2$)</td>
</tr>
<tr>
<td></td>
<td>$1.533$ ($d = 300 \mu$m; $g = 9.81$ m/s$^2$)</td>
</tr>
<tr>
<td></td>
<td>$0.0597$ ($d = 75 \mu$m; $g = 2.45$ m/s$^2$)</td>
</tr>
<tr>
<td></td>
<td>$65$ ($d = 75 \mu$m; $g = 9.81$ m/s$^2$)</td>
</tr>
<tr>
<td></td>
<td>$286$ ($d = 150 \mu$m; $g = 9.81$ m/s$^2$)</td>
</tr>
<tr>
<td></td>
<td>$799$ ($d = 300 \mu$m; $g = 9.81$ m/s$^2$)</td>
</tr>
<tr>
<td></td>
<td>$19$ ($d = 75 \mu$m; $g = 2.45$ m/s$^2$)</td>
</tr>
<tr>
<td>Froude number; $Fr_p = \frac{v_t^2}{(gd)}$</td>
<td>$8 \times 10^{-10}$ ($d = 75 \mu$m; $A^R = 10^{-19}$ Pa)</td>
</tr>
<tr>
<td></td>
<td>$8 \times 10^{-9}$ ($d = 75 \mu$m; $A^R = 10^{-18}$ Pa)</td>
</tr>
<tr>
<td></td>
<td>$3.2 \times 10^{-8}$ ($d = 75 \mu$m; $A^R = 4 \times 10^{-18}$ Pa)</td>
</tr>
</tbody>
</table>

Table 4.1: Computational domain and simulation parameters.
Figure 4.1: Snapshots of the particle volume fraction field in a periodic domain. Domain-averaged particle volume fraction ($\phi$) is (a) 0.1 and (b) 0.3. Simulation parameters are listed in table 4.1. Fluidization simulations of non-cohesive particles are performed with $Fr_p = 65$. 
Particle phase stress tensor is expressed using gradients of particle phase velocities, assuming a constitutive relation of the form:

\[ \sigma = [p - \mu_b(\nabla \cdot \mathbf{u}_s)]I - 2\mu_s \mathbf{S}, \]  \hspace{1cm} (4.3)

where \( p \) is pressure, \( \mu_b \) is bulk viscosity, \( \mu_s \) is shear viscosity, and \( \mathbf{S} \) is rate of deformation tensor:

\[ \mathbf{S} = \frac{1}{2} [\nabla \mathbf{u}_s + (\nabla \mathbf{u}_s)^T] - \frac{1}{3}(\nabla \cdot \mathbf{u}_s)I. \]  \hspace{1cm} (4.4)

Based on simulation results, we propose closures for pressure \( p \), bulk viscosity \( \mu_b \), and shear viscosity \( \mu_s \) for both non-cohesive and cohesive particles. In the following, we first illustrate that the present methodology can yield results for non-cohesive particles that are consistent with analytically derived kinetic theory models, and demonstrate the suitability of the methodology (section 4.3.1). Then, we modify these closures to include cohesion (section 4.3.2).
4.3.1 Non-cohesive particles

As shown in table 4.1, fluidization simulations with non-cohesive particles are performed for several Froude numbers corresponding to different values of particle diameter and acceleration due to gravity as well as for different domain-averaged solid volume fraction. In the model development, independent variables and scalings are carefully chosen so that the stress results from these different simulations collapse, ensuring the generality of the proposed model.

Pressure

From equation (4.3), we have

\[
\frac{1}{3} \text{tr}(\sigma) = p - \mu_b \nabla \cdot \mathbf{u}_s. \tag{4.5}
\]

As detailed in section 4.2, \(\sigma\) is computed for each computational cell, and \(\text{tr}(\sigma)\) is binned with solid volume fraction \(\phi\), granular temperature \(T\), and rate of dilation \(\nabla \cdot \mathbf{u}_s\).

Figure 4.3 shows the dimensionless trace of stress tensor \(\frac{1}{3} \text{tr}(\sigma)/(\rho_s v_t^2)\) versus the dimensionless rate of dilation \(d(\nabla \cdot \mathbf{u}_s)/v_t\) for two combinations of solid volume fraction \(\phi\) and dimensionless granular temperature \(T/v_t^2\). It is found that \(\text{tr}(\sigma)\) exhibits an linear relationship with \(\nabla \cdot \mathbf{u}_s\) for both \(\nabla \cdot \mathbf{u}_s < 0\) and \(\nabla \cdot \mathbf{u}_s > 0\) segments. This finding is consistent with equation (4.5), and thus supports the suitability of the constitutive equation (4.3). Furthermore, since \(\text{tr}(\sigma)\) varies substantially with \(\nabla \cdot \mathbf{u}_s\) in the system, the pressure \(p\) is extracted from bins where \(\nabla \cdot \mathbf{u}_s \sim 0\). This result also suggests that dilation/compaction effects can be substantial in gas-fluidization of particles, and should be accounted for in two-fluid model simulations.
Figure 4.3: Dimensionless trace of stress tensor vs dimensionless rate of dilation for two combinations of solid volume fraction and granular temperature. In both cases, $\text{tr}(\sigma)$ exhibits a linear relationship with $\nabla \cdot u_s$ for both $u_s < 0$ and $u_s > 0$ segments as indicated by the dashed lines. Data from fluidization simulations of non-cohesive particles; $Fr_p = 799; \langle \phi \rangle = 0.1$.

Figure 4.4(a) shows the variation of $p/(\rho_s v_t^2)$ with $T/v_t^2$. It is found that $p$ scales with $T$, which is consistent with the standard kinetic theory [25],

$$p = \rho_s H(\phi) T,$$

$$H(\phi) = \phi[1 + 4\eta \phi g_0],$$

where $\eta = (1 + e_p)/2$ and $g_0$ is the radial distribution function at contact.

Figure 4.4(b) shows a plot of $p/(\rho_s T)$ against $\phi$ for various $Fr_p$ and $\langle \phi \rangle$. The data collapse onto a single curve, and it is found that the standard kinetic theory captures the collapse well. Throughout the present study, we have used $g_0$ proposed by Chialvo et al. [28]:

$$g_0 = \frac{1 - \phi/2}{(1 - \phi)^3} + \frac{\alpha g_0 \phi^2}{(\phi_c - \phi)^{3/2}},$$

$$\phi_c$$
Figure 4.4: (a) Dimensionless pressure vs dimensionless granular temperature for various solid volume fractions. In all cases, $p$ scales with $T$ as indicated by the dashed line with slope of 1. Data from fluidization simulations of non-cohesive particles; $F_{rp} = 65; \langle \phi \rangle = 0.1$. (b) Pressure scaled by granular temperature vs solid volume fraction for various Froude numbers and domain-averaged solid volume fractions. Dashed line: equation (4.6).

where $\alpha_{g0} = 0.58$, and $\phi_c$ is a jamming volume fraction that varies with the sliding friction coefficient $\mu_p$ [28, 52, 90]. The jamming condition was found by Sun and Sundaresan [90] to depend on the nature of the deformation. Simple shear appears to afford the smallest value of $\phi_c$ among all types of deformations. For $\mu_s = 0.5$, simple shear simulations yielded $\phi_c = 0.587$ [52]. In the present simulations, where appreciable compaction and dilation are also at play, $\phi_c = 0.61$ was found to fit the data better and is used in all subsequent figures.

**Bulk viscosity**

According to equation (4.5) as well as figure 4.3, bulk viscosity $\mu_b$ can be found by computing the slope of $\frac{1}{3} \text{tr}(\sigma)$ versus $-\nabla \cdot u_s$. As indicated in the figure, the slope differs between $\nabla \cdot u_s < 0$ and $\nabla \cdot u_s > 0$. Thus, $\mu_b$ is calculated for $\nabla \cdot u_s < 0$ (corresponding to compaction) and $\nabla \cdot u_s > 0$ (corresponding to dilation) separately.
Figure 4.5(a) shows the dimensionless bulk viscosity $\mu_b/(\rho_s dvt)$ versus $T/v_t^2$ for two solid volume fractions. It is found that $\mu_b$ scales with $\sqrt{T}$, which is consistent with the standard kinetic theory. According to [25]

$$\mu_b = \left(\frac{\eta}{3\sqrt{\pi}}\phi^2 g_0\right)\rho_s d\sqrt{T}.$$  \hspace{1cm} (4.9)

However, unlike the standard kinetic theory, it is found that bulk viscosity is path-dependent, and bulk viscosity is larger for compaction than for dilation for a given solid volume fraction and granular temperature. This path dependence of bulk viscosity has also been observed in simulations of traveling waves in particle-fluid suspensions [184, 185].

We plot the bulk viscosity scaled by granular temperature, $\mu_b/(\rho_s d\sqrt{T})$, against $\phi$ for different Froude number $Fr_p$ and $\langle \phi \rangle$ in figure 4.5(b). Values of bulk viscosity for compaction and those for dilation each collapse. The bulk viscosity data could be captured by

$$\mu_b = (\alpha_{\mu_b}\eta\frac{8}{3\sqrt{\pi}}\phi^2 g_0)\rho_s d\sqrt{T},$$  \hspace{1cm} (4.10)

where $\alpha_{\mu_b} = 1$ for dilation and $\alpha_{\mu_b} = 1.5$ for compaction.

**Shear viscosity**

The shear viscosity, $\mu_s$, is calculated as:

$$\mu_s = \frac{\tau : (2S)}{(2S) : (2S)},$$  \hspace{1cm} (4.11)

where deviatoric stress tensor $\tau = -\sigma + \frac{1}{3}\text{tr}(\sigma)I$.

Kinetic-theory-based models derived for gas-solid systems [18, 162–168] have taken into consideration the potential influence of slip velocity $u_{\text{slip}} = |u_p - u_s|$ on shear viscosity. Therefore,
in our analysis, $\mu_s$ was computed in each Eulerian grid, and initially binned with $u_{\text{slip}}$, $\phi$, and $T$. Figure 4.6 shows the dimensionless shear viscosity $\mu_s/(\rho_s dv_t)$ versus $T/v_t^2$ for various dimensionless slip velocities $u_{\text{slip}}/v_t$. Two regimes are readily identified as indicated by the dashed lines, where $\mu_s$ scales with $T$ in the low $T$ regime and with $T^{1/2}$ in the high $T$ regime. These two flow regimes are also observed in the kinetic-theory-based models derived for gas-solid systems [18, 162–168]. However, unlike these studies, it is found that $u_{\text{slip}}$ affects $\mu_s$ minimally. Therefore, $\mu_s$ was simply binned with $\phi$ and $T$.

We plot the scaled shear viscosity in the high $T$ regime $\mu_{s,c}/(\rho_s d\sqrt{T})$ against $\phi$ for various $Fr_p$ and $\langle \phi \rangle$ in figure 4.7(a). The data are consistent with the predictions of standard kinetic theory that does not account for effects of interstitial fluid [25]:

$$
\mu_{s,c} = \left(\frac{2 + \alpha_0}{6}\right) \left[ \frac{5\sqrt{\pi}}{48g_0\eta(2-\eta)} \left( 1 + \frac{8}{5} \phi \eta g_0 \right) \left( 1 + \frac{8}{5} \eta (3\eta - 2) \phi g_0 \right) + \frac{16}{5} \eta \phi \eta^2 g_0 \right] \rho_s d \sqrt{T},
$$

(4.12)
where $\alpha_0 = 1.6$. The modified kinetic theory proposed by Chialvo et al. [28] that is based on inertial number model in the dense regime [69–71] yields essentially indistinguishable predictions as equation (4.12), as illustrated in figure 4.7(a). This consistency again affirms the validity of the computational approach followed in the present study.

We found that shear viscosity data in the low $T$ regime could be captured as,

$$\mu_{s,g} = f_{\mu_s} \phi \rho_s T \sqrt{d/g}. \quad (4.13)$$

Figure 4.7(b) shows a plot of $\frac{\mu_s}{\rho_s \sqrt{d/g}}$ against $\phi$ extracted from simulations performed using different particle diameters and acceleration due to gravity (which are combined in terms of Froude number). Data collapse reasonably well onto a single curve, supporting the scaling. The dashed line in Figure 4.7(b) correspond to

$$f_{\mu_s} = \alpha_{\mu_s} \phi^2, \quad (4.14)$$

where $\alpha_{\mu_s} = 8.0$.

The transition from the high $T$ regime to the low $T$ regime can be understood as a change in time between inter particle collisions. It is assumed that $\mu_s \sim \rho_s T \tau$, where $\tau$ is a collision time for the system. At high $T$ conditions, the collision time scales as $\sqrt{d/g}$. In the low $T$ regime, collisions appear to be largely determined by gravitational fall and hence the $\sqrt{d/g}$ scaling for collision time.

In our computationally generated model approach, we simply bridge the low and high $T$ regimes via

$$\mu_s = \min(\mu_{s,g}, \mu_{s,c}). \quad (4.15)$$

As shown in figure 4.8, the equation captures both regimes reasonably well.
Figure 4.6: Dimensionless shear viscosity vs dimensionless granular temperature for various dimensionless slip velocities and $\phi = 0.465$. Two regimes are identified. $\mu_s$ scales with $T$ in the low $T$ regime and with $T^{1/2}$ in the high $T$ regime, as indicated by the two dashed lines with slope of 1 (left) and 1/2 (right). Data from fluidization simulations of non-cohesive particles; $Fr_p = 286; \langle \phi \rangle = 0.3$.

Figure 4.7: Scaled shear viscosity vs solid volume fraction for different Froude numbers and domain-averaged solid volume fractions. (a) Data in the high $T$ regime where $\mu_s$ scales with $T^{1/2}$ are plotted. Dashed line: equation (4.12). Dotted line: the modified kinetic theory proposed by Chialvo et al. [28]. (b) Data in the low $T$ regime where $\mu_s$ scales with $T$ are plotted. Dashed line: equation (4.14).
Figure 4.8: Dimensionless shear viscosity vs dimensionless granular temperature for various solid volume fractions. Data from fluidization simulations of non-cohesive particles; $Fr_p = 65$; $<\phi> = 0.3$. Solid lines: equations (4.12), (4.13), and (4.15).

**Pseudo-thermal energy balance**

As proposed kinetic-theory-based models for pressure, bulk viscosity, and shear viscosity directly depend on granular temperature, a balance of pseudo-thermal energy (PTE) of particle velocity fluctuations needs to be solved to obtain granular temperature. In fluidized gas-particle mixtures, the rate of production of PTE by shear $-\sigma : \nabla u_s$ is, to a good approximation, balanced locally by the rate of dissipation of PTE by interparticle collisions $J_{\text{coll}}$. Thus, we set

$$-\sigma : \nabla u_s = J_{\text{coll}}.$$  \hspace{1cm} (4.16)

This approximation is supported by the following two observations.

First, our computational results show that $u_{\text{slip}}$ affects $-\sigma : \nabla u_s$ minimally, and thus all the terms that depend on $u_{\text{slip}}$ affect the rates of generation and dissipation of PTE only in a secondary fashion (over the wide parameter range we probed). Hence any terms involving $u_{\text{slip}}$ cannot be probed using our results. The weak role of $u_{\text{slip}}$ is illustrated in figure 4.9, where the scaled rate of production of PTE by shear $\frac{-\sigma : \nabla u_s}{\rho \nu_l^3}$ is plotted against $T/v_l^2$ for various $u_{\text{slip}}/v_l$. 

127
Second, at high $T$ regime, the expression for $J_{\text{coll}}$ from kinetic theory of granular materials is found to match $-\sigma : \nabla u_s$ from simulations. This is illustrated in figure 4.10(a) where the scaled rate of production of PTE by shear $-\sigma : \nabla u_s \frac{d}{\rho_s \sqrt{T}}$ is plotted against $\phi$ for various $Fr_p$ and $\langle \phi \rangle$. Data collapse onto a single curve, which is described well by equation (4.16) and $J_{\text{coll}}$ from modified kinetic theory [28]:

$$J_{\text{coll}} = \frac{12}{\sqrt{\pi}} \phi^2 g_0(1 - e_{\text{eff}}^2) \frac{\rho_s T^{3/2}}{d}. \quad (4.17)$$

In this equation, the restitution coefficient $e_p$ in the standard kinetic theory [25] is replaced by an effective restitution coefficient $e_{\text{eff}}$ [28] to account for the total energy loss due to inelasticity and friction during an interparticle collision, which is supported by analytical derivations of kinetic theory for slightly frictional particles [186]. Based on simple shear simulations of frictional particles, Chialvo et al. [28] related $e_{\text{eff}}$ to the particle sliding friction coefficient $\mu_p$ as the following,

$$e_{\text{eff}} = e_p - \frac{3}{2} \mu \exp(-3\mu). \quad (4.18)$$

Both observations above suggest that the approximation $-\sigma : \nabla u_s = J_{\text{coll}}$ is reasonable, and therefore we formulate models for $J_{\text{coll}}$ based on $-\sigma : \nabla u_s$ data from simulations, when equation (4.17) is not valid (e.g., as in the low $T$ regime).

It is useful to express equation (4.17) as

$$J_{\text{coll}} = f_J(\phi) \frac{\rho_s T}{\tau_{\text{vis}}}, \quad (4.19)$$

where $\tau_{\text{vis}} = \frac{\sigma \rho_s}{\mu_s}$. Following the definitions of $\mu_s$ in section 4.3.1, at high $T$ regime, $\mu_s \sim \rho_s d \sqrt{T}$. This leads to

$$J_{\text{coll,c}} = f_{J,c}(\phi) \frac{\rho_s T^{3/2}}{d}, \quad (4.20)$$
and as in equation (4.17),
\[ f_{J,c}(\phi) = \frac{12}{\sqrt{\pi}} \phi^2 g_0 (1 - e_{\text{eff}}^2). \]  
(4.21)

At low $T$ regime, where $\mu_s \sim \rho_s T \sqrt{d/g}$, we then anticipate
\[ J_{\text{coll},g} = f_{J,g}(\phi) \rho_s T^2 \frac{d^2}{g}. \]  
(4.22)

If this model is reasonable, rate of production of PTE by shear in the low $T$ regime, scaled as \( \sigma \cdot \nabla u \cdot \frac{d^2}{g} \), should only be a function of $\phi$ independent of Froude number of the particles used in the simulations. Figure 4.10(b) confirms that the data do collapse reasonably well, supporting the model form chosen in equation (4.22). The dashed line in this figure corresponds to
\[ f_{J,g}(\phi) = \alpha_{J,g} \phi^2 g_0 (1 - e_{\text{eff}}^2), \]  
(4.23)
where $\alpha_{J,g} = 45$.

As in the case of shear viscosity, we bridge $J_{\text{coll}}$ in the low and high $T$ regimes via
\[ J_{\text{coll}} = \min(J_{\text{coll},g}, J_{\text{coll},c}). \]  
(4.24)

As shown in figure 4.11, this equation captures both regimes reasonably well.

**Conclusion**

At high $T$ regime, it is found that the results for non-cohesive particles in the high $T$ regime obtained by post-processing CFD-DEM simulations agree well with constitutive expressions afforded by the kinetic theory of granular materials, which have been modified to include the effect of inter-particle friction. These findings demonstrate the validity of the adopted methodology. The present computational approach has also revealed a low $T$ regime, where
Figure 4.9: Dimensionless production rate of PTE by shear vs dimensionless granular temperature for various dimensionless slip velocities and \( \phi = 0.465 \). Two regimes are identified. \(-\sigma : \nabla u_s\) scales with \( T^2 \) in the low \( T \) regime and with \( T^{3/2} \) in the high \( T \) regime, as indicated by the two dashed lines with slope of 2 (left) and 3/2 (right). Data from fluidization simulations of non-cohesive particles; \( Fr_p = 286; \langle \phi \rangle = 0.3 \).

Figure 4.10: Rescaled rate of production of PTE by shear scaled vs solid volume fraction for different Froude numbers and domain-averaged solid volume fractions. (a) Data in the high \( T \) regime where \(-\sigma : \nabla u_s\) scales with \( T^{3/2} \) are plotted. Dashed line: equation (4.21). (b) Data in the low \( T \) regime where \(-\sigma : \nabla u_s\) scales with \( T^2 \) are plotted. Dashed line: equation (4.23).
Figure 4.11: Dimensionless production rate of PTE by shear vs dimensionless granular temperature for various solid volume fractions. Data from fluidization simulations of non-cohesive particles; $Fr_p = 65; \langle \phi \rangle = 0.3$. Solid lines: equations (4.20) (4.22) and (4.24).

the inter-particle collision time is determined by gravitational fall between collisions. Modifications to the kinetic theory constitutive models are proposed to capture both the low and high $T$ regimes.

### 4.3.2 Cohesive particles

For cohesive particles, interparticle van der Waals forces are included. As shown in table 4.1, simulations are performed with two Hamaker constants, and the cohesion strength is characterized by the modified Bond number $Bo^* = \frac{F_{coh}^{max}}{d^2 Y R} = \frac{AR}{(24s_{min}^R d Y R)}$. Here, $F_{coh}^{max}$ is the maximum cohesive force in the system. From equation (3.10), for $s = s_{min}^R \ll d$, $F_{coh}^{max}$ becomes:

$$F_{coh}^{max} = F_{vdw}(A^R, s_{min}^R) = \frac{ARd}{24s_{min}^R d^2}.$$  \hspace{1cm} (4.25)

In the following, kinetic-theory-based models for cohesive particles have been carefully proposed to ensure that (1) for the case of Hamaker constant being zero, the models return
back to the ones proposed in section 4.3.1, and (2) model would collapse simulation results from different cohesion levels.

**Pressure**

From previous studies [58, 89] and the results in Chapter 2, it is found that cohesion bifurcates the the inertial regime (Bagnold scaling) into two regimes: a new rate-independent regime (namely cohesive regime) at low shear rates and an inertial regime at high shear rates, where no changes occur from cohesion. Such effects are also observed in the results here as shown in figure 4.12, where it is found that with cohesion pressure results are unchanged in the high $T$ regime and $P$ scales with $T$ but a plateau emerges at low $T$ regime due to cohesion.

This plateau region at lower $T$ regime, which corresponds to solid-like behavior of particles, forms because that particles start to form agglomerates due to cohesion. To illustrate, we study the average coordination number $Z$, which is defined as the average number of contacts per particle in the region of interest. We calculate $Z$ for each cell, and bin the results with $\phi$ and $T$, as shown in figure 4.13. Two trends are observed. First, for a given $\phi$, $Z$ decreases with increasing $T$; this behavior corresponds to that increasing agitation of the particles would eventually break up the agglomerates of particles. Second, for a given temperature in the low temperature region, $Z$ increases but quickly saturates with increasing $\phi$; this behavior is consistent with that particles would contact more with increased concentration, but would eventually saturate due to geometric constraint. This microstructure has also been observed previously [58, 89] and in Chapter 2. This consistency in the regime transition manifested in both macroscopic quantity ($p$) and microstructure ($Z$) again affirms the validity of the methodology in this study.

However, different from these previous studies of cohesive particles [58, 89] and the study of Chapter 2, the present methodology allows for examining stress results at a wider parameter
space. Specifically, we can now study lower solid volume fractions at lower temperature regime, which have been difficult to access \[89\]. The results for this region are shown in figure 4.14. In this figure, to study the effects of cohesion, we subtract the contribution from collisions that is present for non-cohesive particles \( \rho_s H(\phi)T \) from the total pressure \( p \). We focus on the low temperature region where pressure is essentially temperature-independent. One can see that as \( \phi \) increases, \( p - \rho_s H(\phi)T \) starting from 0, initially decreases to become negative, and then increases.

This non-monotonic behavior at low temperature region can be understood physically as the following. At low temperature region, effects from cohesion dominate over particle agitation. These effects from cohesion are manifested differently depending on the number of particles present locally. At low solid volume fractions \( (\phi < 0.2) \), there are not enough particles to form agglomerates (see figure 4.13). Attractive van der Waals forces between particles would result in a negative pressure. At high solid volume fractions \( (\phi > 0.2) \), particles form agglomerates which allow for percolation (see figure 4.13) that induces an increase in pressure.

To model this non-monotonic behavior at low temperature region, at low solid volume fraction, \( p - \rho_s H(\phi)T \) is found to scale with \( \phi^2 \), which is consistent with van der Waals equation of state. We then propose the following:

\[
\frac{d^2}{F_{\text{coh}}}(p - \rho_s H(\phi)T) = -\alpha_{\text{coh,1}}\phi^2 \quad \text{for} \quad \phi < \phi_a.
\]

(4.26)

Here, \( \phi_a = 0.2 \) and \( \alpha_{\text{coh,1}} = 0.003 \). As shown in figure 4.14, this equation denoted by solid line captures the data of \( \phi < 0.2 \). For high solid volume fraction, to capture the increase of pressure due to percolation, we add a new term that is consistent the study of Chapter 2 on the right-hand side:

\[
\frac{d^2}{F_{\text{coh}}}(p - \rho_s H(\phi)T) = -\alpha_{\text{coh,1}}\phi^2 + \alpha_{\text{coh,2}} \frac{(\phi - \phi_a)^2}{\phi_c - \phi} \quad \text{for} \quad \phi \geq \phi_a.
\]

(4.27)
Figure 4.12: Dimensionless pressure vs dimensionless granular temperature for various solid volume fractions. Data from fluidization simulations of cohesive particles; $Bo^* = 8 \times 10^{-9}$ in (a) and $Bo^* = 8 \times 10^{-10}$ in (b); $Fr_p = 65; (\phi) = 0.3$. Solid lines: equation (4.28).

Here, $\alpha_{coh,2} = 0.0034$. As shown in figure 4.14, this equation denoted by dashed line captures the data of $\phi > 0.2$.

Assembling these models together, we obtain the following:

$$p = \left\{ \begin{array}{ll}
\rho_s \phi [1 + 2(1 + e_p) \phi] T - \alpha_{coh,1} \frac{F_{coh}^{max}}{d^2} \phi^2 & \text{for } \phi < \phi_a \\
\rho_s \phi [1 + 2(1 + e_p) \phi] T - \alpha_{coh,1} \frac{F_{coh}^{max}}{d^2} \phi^2 + \alpha_{coh,2} \frac{F_{coh}^{max}}{d^2} \frac{(\phi - \phi_a)^2}{(\phi_c - \phi)} & \text{for } \phi \geq \phi_a
\end{array} \right.$$  \hspace{1cm} (4.28)

where $\alpha_{coh,1} = 3.9 \times 10^{-3}$, $\alpha_{coh,1} = 3.9 \times 10^{-3}$, $\phi_a = 0.2$, and $\phi_c = 0.61$. As shown in figures 4.12(a-b) and 4.14, the model captures the pressure data for all cohesion levels.

For bulk viscosity, it is found that the inclusion of cohesion has negligible impact on the values, and thus equation (4.10) is applied.
Figure 4.13: Average coordination number vs dimensionless granular temperature for various solid volume fractions. Data from fluidization simulations of cohesive particles; $Bo^* = 8 \times 10^{-9}$; $Fr_p = 65$; $\langle \phi \rangle = 0.3$.

Figure 4.14: Scaled pressure contributed from cohesion vs solid volume fraction. Solid line: equation (4.26). Dashed line: equation (4.27)
Shear viscosity

As shown in figures 4.15(a-c) where dimensionless shear stress ($\tau \equiv \mu \dot{\gamma}$) for both non-cohesive (as in (a)) and cohesive particles (as in (b-c)) is plotted against dimensionless granular temperature for different solid volume fractions, similar to pressure, shear stress ($\tau \equiv \mu_s \dot{\gamma}$, $\dot{\gamma} \equiv \sqrt{2S : S}$) for cohesive particles is unchanged with cohesion at high $T$ regime, but becomes temperature-independent at low $T$ limit. This behavior is consistent with previous findings [89] as well as the results in Chapter 2, and again supports the validity of the present methodology.

In the transition between these two regimes, one can observe a dip in shear stress. Physically, it corresponds to that the agglomerates are broken up by increased particle agitation, inducing in a drop in shear stress. To study this dip and low temperature region, in figure 4.16(a), we subtract the contribution from collisions that is present for non-cohesive particles $\mu^*_s = \min(\mu_{s,g}, \mu_{s,c})$ from overall shear viscosity and plot for low temperatures. In this figure, one can readily observe the dependence of $(\mu - \mu^*)$ on granular temperature.

To capture this dependence, based on the fluidity approach of Picard et al. [187], Irani et al. [89] derives a model to bridge the two $T$ limits as shown below,

$$
\mu \dot{\gamma} = \mu^*_s \dot{\gamma} + \tau_y \frac{W(x)}{x}.
$$

(4.29)

Here, $\tau_y$ is the yield stress, and $\mu^*_s = \min(\mu_{s,g}, \mu_{s,c})$ corresponds to the model for non-cohesive particles. $W(x)$ is the Lambert-W function, which is defined as $W^{-1}(z) = z \exp(z)$. For computation, its principal branch ($x > 0$) can be approximated [188] as $W(x) \approx [2 \ln(1 + 0.8842y) - \ln(1 + 0.9294 \ln(1 + 0.5106y)) - 1.213]/[1 + 1/(2 \ln(1 + 0.8842y) + 4.688)]$, where $y = \sqrt{2ex + 2}$. Here, $e$ is Napier’s constant. As detailed by Irani et al. [89], the underlying physics of the model is the competition between kinetic energy supplied by shearing and
the cohesive energy, as captured by $\frac{W(x)}{x}$. Correspondingly, $x$ is assumed to be $f_1(\phi)\frac{\rho_s T d^2}{F_{\text{coh}}^\text{max}}$. Similar to the one for pressure, it is assumed that the yield stress $\tau_y$ has the form of $\tau_y = f_2(\phi)\frac{F_{\text{coh}}^\text{max}}{d^2}$.

Thus, equation (4.29) becomes,

$$f_2(\phi) = d^2 \frac{F_{\text{coh}}^\text{max}}{W(f_1(\phi)\frac{\rho_s T d^2}{F_{\text{coh}}^\text{max}})}(\mu s^* - \mu^s)\dot{\gamma}.$$

(4.30)

To obtain values of $f_1(\phi)$, for each $\phi$ value, we pick two temperatures and equate the right-hand side of equation (4.30) for these two cases. We can then obtain the value of $f_1(\phi)$ for each $\phi$ value. The results based on temperatures in figure 4.16(a) are shown in the insert of figure 4.16(b). One can see that points are collapsed onto a single curve, indicating the validity of the equation form from fluidity approach. Furthermore, this curve can be described by the following model, as denoted by the solid line in the figure:

$$f_1(\phi) = \psi_1 \frac{\phi_c - \phi}{\phi},$$

(4.31)

where $\psi_1 = 2.23 \times 10^4$.

Combining equations (4.30) and (4.31), we can evaluate $f_2(\phi)$ by computing $\frac{x}{W(x)}\frac{d^2}{F_{\text{coh}}^\text{max}}(\mu s^* - \mu^s)\dot{\gamma}$ as in figure 4.16(b). One can see that, compared to figure (a), with $\frac{x}{W(x)}$ from fluidity approach data points from different temperatures are now collapsed onto a single curve. This collapse can be described the following model, as denoted by the solid line in the figure:

$$f_2(\phi) = \psi_2 \frac{\phi}{\phi_c - \phi},$$

(4.32)

where $\psi_2 = 4.84 \times 10^{-4}$. 
Assembling these equations together, we have the following expression for $x$:

$$x = \psi_1 \phi_c - \phi \frac{\rho_s T d^2}{F_{\text{coh}}^{\text{max}}} = \psi_1 \psi_2 \frac{\rho_s T}{\psi_2 \phi_c - \phi} = \psi_1 \psi_2 \frac{\rho_s T}{\tau_y} = \alpha_{W,1} \frac{\rho_s T}{\tau_y},$$

where $\alpha_{W,1} = \psi_1 \psi_2 = 10.8$.

Thus, we have the final shear viscosity model for cohesive particles:

$$\mu = \mu_s^* + \frac{\tau_y}{\dot{\gamma}} W(\alpha_{W,1} \frac{\rho_s T}{\tau_y}),$$

where $\tau_y = \alpha_{\text{coh},2} \frac{F_{\text{coh}}^{\text{max}}}{d^2} \phi_c - \phi$, $\alpha_{\text{coh},2} = \psi_2 = 4.84 \times 10^{-4}$, and $\alpha_{W,1} = 10.8$.

To explicitly illustrate the ability of fluidity model to capture the dip in the shear stress, comparisons between model predictions using equation (4.34) and simulation results for shear stress are shown in figures 4.15(a-c). In the figures, the unfilled symbols are simulation results, and filled symbols are model predictions from equation (4.34). As shown in figures, this equation captures all the regimes as well as the transitions between them.

It should be noted that this yield-stress based model for cohesive particles is consistent with prior observations from both experiments and simulations. For fluidization of Geldart Group A particles [9], for which interparticle van der Waals forces start to become important compared to particle weight, a bubbleless expanded regime is observed in both experiments [9, 155] and simulations [111] (also the study on fines in Chapter 3). Both experiments [9, 155] and simulations [111] found that particles are in a completely static state in this regime. This regime corresponds to the case where the shear stress supplied in the system does not overcome the yield stress $\tau_y$. Furthermore, it has been found in these experimental and simulation studies that the formation of this regime depends on solid volume fraction of the system, which corresponds to the dependence of $\tau_y$ on solid volume fraction $\phi$. 

138
Figure 4.15: Dimensionless shear stress vs dimensionless granular temperature for various solid volume fractions. Unfilled (filled) symbols are simulation results (model predictions from equations (4.12) (4.13), and (4.34)). Data from fluidization simulations of both (a) non-cohesive particles and (b-c) cohesive particles; $Bo^* = 8 \times 10^{-9}$ in (b) and $Bo^* = 8 \times 10^{-10}$ in (c); $Fr_p = 65$; $\langle \phi \rangle = 0.3$.

Figure 4.16: Shear viscosity subtracted by the component corresponding for non-cohesive particles vs solid volume fraction for different temperatures. Data from fluidization simulations of cohesive particles; $Bo^* = 8 \times 10^{-9}$; $Fr_p = 65$; $\langle \phi \rangle = 0.3$. Data from (a) are rescaled in main figure of (b) through $x/W(x)$, where $x = f_1(\phi)\frac{\rho_s T d^2}{\rho_{coh}}$. $f_1$ is computed and plotted in the insert of (b). Solid line in the main figure of (b): equation (4.32). Solid line in the insert of (b): equation (4.31).
Pseudo-thermal energy balance

As shown in figure 4.17, similar to results to pressure and shear viscosity, production rate of PTE by shear for cohesive particles is unchanged at high $T$ regime. At low $T$ regime, it is increased, and scales with $\sqrt{T}$. It can be explained by that dissipation of PTE by interparticle collisions is enhanced by an additional dissipation mechanism due to interparticle cohesion. It is assumed that both mechanisms are additive. Thus, equation (4.16) proposed for non-cohesive particles is now the following,

$$-\sigma : \nabla u_s = J_{\text{coh}} + J_{\text{coll}},$$

(4.35)

where $J_{\text{coh}}$ is the dissipation rate of PTE due to interparticle cohesion. $J_{\text{coh}}$ is assumed to have a scaling similar to $J_{\text{coll}}$, as $J_{\text{coh}} \sim \rho_s T/\tau_{\text{vis}} \sim T \mu_s$. From section 4.3.2, it is found that in this regime, $\mu_s \equiv \tau/\gamma \sim \frac{\tau d}{\sqrt{T}} \sim \tau_y \frac{W(\alpha_{W,2} \rho_s T_\gamma)}{\alpha_{W,2} \rho_s T_\gamma} \frac{d}{\sqrt{T}}$. Thus, $J_{\text{coh}} \sim \tau_y \frac{W(\alpha_{W,2} \rho_s T_\gamma)}{\alpha_{W,2} \rho_s T_\gamma} \sqrt{T}$. 

Correspondingly, the following model is proposed,

$$J_{\text{coh}} = \alpha_{\text{coh},3} \tau_y W(\alpha_{W,2} \rho_s T_\gamma) \frac{\sqrt{T}}{\alpha_{W,2} \rho_s T_\gamma} \frac{d}{\sqrt{T}}$$

(4.36)

Combing equations (4.24) (4.35), and (4.36) results in the following PTE balance for cohesive granular materials:

$$-\sigma : \nabla u_s = \alpha_{\text{coh},3} \tau_y \frac{W(\alpha_{W,2} \rho_s T_\gamma) \sqrt{T}}{\alpha_{W,2} \rho_s T_\gamma} \frac{d}{\sqrt{T}} + \min(J_{\text{coll,g}}, J_{\text{coll,c}}),$$

(4.37)

where $\alpha_{\text{coh},3} = 1.65$ and $\alpha_{W,2} = 3.87$. As shown in figure 4.17(a-b), this equation captures all the regimes as well as the transitions between them. Furthermore, it should be noted that it works for different cohesion levels without additional changes to model parameters.
Constitutive equation

\[ \boldsymbol{\sigma} = [p - \mu_b (\nabla \cdot \mathbf{u}_s)] \mathbf{I} - 2 \mu_s \mathbf{S}, \]

\[ \mathbf{S} = \frac{1}{2} \left[ \nabla \mathbf{u}_s + (\nabla \mathbf{u}_s)^T \right] - \frac{1}{3} (\nabla \cdot \mathbf{u}_s) \mathbf{I}. \]

Radial distribution function at contact

\[ g_0 = \frac{1 - \phi/2}{(1 - \phi)^2} + \frac{\phi_0 \phi^2}{(\phi_1 \phi - \phi_0)^{1/2}} \]

Effective restitution coefficient

\[ e_{\text{eff}} = e_p - \frac{3}{2} \mu \exp(-3 \mu); \quad (e_{\text{eff}} = 0.733 \text{ for } \mu = 0.5) \]

Non-cohesive particles

Pressure

\[ p = \rho_s \phi \left[ 1 + 4 \eta \phi g_0 \right] T; \quad \eta = (1 + e_p)/2 \]

Bulk viscosity

\[ \mu_b = \begin{cases} 
\alpha_{p, \text{com}} \eta \frac{8}{3 (1 - \phi)} \phi^2 g_0 \rho_s d \sqrt{T}, & \text{for } \nabla \cdot \mathbf{u}_s < 0 \\
\alpha_{p, \text{dil}} \eta \frac{8}{3 (1 - \phi)} \phi^2 g_0 \rho_s d \sqrt{T}, & \text{for } \nabla \cdot \mathbf{u}_s \geq 0.
\end{cases} \]

Shear viscosity

\[ \mu_s = \min(\mu_{s,g}, \mu_{s,c}) \]

\[ \mu_{s,g} = \alpha_{s,g} \phi_0 \phi^2 \rho_s T \sqrt{d/g}; \quad \mu_{s,c} = \frac{\sqrt{2}}{\phi_0 \phi^2 g_0 (1 - e_{\text{eff}}^2) \rho_s T^{\phi_1 g_0}} \]

Pseudo-thermal energy balance

\[ -\boldsymbol{\sigma} \cdot \nabla \mathbf{u}_s = \min(J_{\text{coll,g}}, J_{\text{coll,c}}) \]

\[ J_{\text{coll,g}} = \alpha_{s,g} \phi_0 \phi^2 g_0 (1 - e_{\text{eff}}^2) \rho_s T^{\phi_1 g_0} d \sqrt{d/g}; \quad J_{\text{coll,c}} = \frac{\sqrt{2}}{\phi_0 \phi^2 g_0 (1 - e_{\text{eff}}^2) \rho_s T^{\phi_1 g_0}} \]

Cohesive particles

Pressure

\[ p = \begin{cases} 
\rho_s \phi \left[ 1 + 2(1 + e_p) \phi g_0 \right] T - \alpha_{\text{coh,1}} \frac{F_{\text{max}}}{d^2} \phi^2, & \text{for } \phi < \phi_a \\
\rho_s \phi \left[ 1 + 2(1 + e_p) \phi g_0 \right] T - \alpha_{\text{coh,1}} \frac{F_{\text{max}}}{d^2} \phi^2 + \alpha_{\text{coh,2}} \frac{F_{\text{max}}}{d^2} (\phi - \phi_a)^2, & \text{for } \phi \geq \phi_a.
\end{cases} \]

\[ F_{\text{max}} = \frac{\Delta R D}{24 \kappa R_{\text{min}}^2}. \]

Bulk viscosity

\[ \mu_b = \begin{cases} 
\alpha_{p, \text{com}} \eta \frac{8}{3 (1 - \phi)} \phi^2 g_0 \rho_s d \sqrt{T}, & \text{for } \nabla \cdot \mathbf{u}_s < 0 \\
\alpha_{p, \text{dil}} \eta \frac{8}{3 (1 - \phi)} \phi^2 g_0 \rho_s d \sqrt{T}, & \text{for } \nabla \cdot \mathbf{u}_s \geq 0.
\end{cases} \]

Shear viscosity

\[ \mu = \min(\mu_{s,g}, \mu_{s,c}) + \frac{\tau_y}{\gamma} \left[ W(\alpha_{W,1} \frac{\tau_T}{\gamma}) - W(\alpha_{W,1} \frac{\tau_T}{\gamma}) \right], \quad \tau_y \text{ is yield stress, and } \tau_y = \alpha_{\text{coh,2}} \frac{F_{\text{max}}}{d^2} \phi^2 (\phi - \phi) \]

\[ \dot{\gamma} = \sqrt{2} \mathbf{S} : \dot{\mathbf{S}}; \quad W(x) \text{ is the Lambert-W function.} \]

Pseudo-thermal energy balance

\[ -\boldsymbol{\sigma} \cdot \nabla \mathbf{u}_s = \alpha_{\text{coh,3}} \tau_y \frac{W(\alpha_{W,2} \frac{\tau_T}{\gamma}) \sqrt{T}}{\alpha_{W,2} \frac{\tau_T}{\gamma}} d + \min(J_{\text{coll,g}}, J_{\text{coll,c}}). \]

Model parameters ( \( \mu = 0.5 \) and \( e_p = 0.9 \))

\[ \phi_c = 0.61, \quad \alpha_{p, \text{com}} = 1.5, \quad \alpha_{p, \text{dil}} = 1, \quad \alpha_{s, \text{g}} = 8.0, \quad \alpha_0 = 1.6, \quad \alpha_{I, \text{g}} = 45 \]

\[ \alpha_{\text{coh,1}} = 3.9 \times 10^{-3}; \quad \phi_a = 0.2; \quad \alpha_{W,1} = 10.8, \quad \alpha_{\text{coh,2}} = 4.84 \times 10^{-4}, \quad \phi_b = 0 \]

\[ \alpha_{\text{coh,3}} = 1.65, \quad \alpha_{W,2} = 3.87. \]

Table 4.2: Computationally generated kinetic-theory-based models for non-cohesive and cohesive particles proposed in the present study.
Figure 4.17: Dimensionless rate of production of PTE by shear vs dimensionless granular temperature for various solid volume fractions. Data from fluidization simulations of cohesive particles; $Bo^* = 8 \times 10^{-9}$ in (a) and $Bo^* = 8 \times 10^{-10}$ in (b); $Fr_p = 65$; $\langle \phi \rangle = 0.3$. Solid lines: equations (4.20) (4.22) (4.37).

Summary

It is found that the stress terms have similar response to the inclusion of cohesion. When particles become cohesive, no changes occur at high $T$ regime. Changes are observed at low $T$ region, and this region is expanded in terms of $T$ covered as cohesion level is increased. These effects of cohesion are consistent with previous findings [58, 89] as well as the results in Chapter 2. At the low $T$ region, a plateau emerges for pressure and shear stress, and the dissipation rate of PTE is enhanced. The transition between these two regimes can be captured by fluidity approach that describes the interplay between the cohesive energy and kinetic energy from particle agitation. Corresponding modifications are made to the models for non-cohesive particles to account for the changes.
4.4 Conclusions

In this study, we introduced a methodology through which one can propose a model for particle phase stress based on CFD-DEM simulations. To substantiate this methodology, we performed fluidization of both non-cohesive particles and particles with van der Waals forces. Based on the simulation results, closures for pressure, bulk viscosity, shear viscosity, as well as for the pseudo-thermal energy balance are proposed. For non-cohesive particles, the present methodology generates models that are consistent with the analytically derived kinetic theory models, confirming the validity of the methodology. In addition, the present methodology uncovers features of particle phase stress that are not observed before. For particles with van der Waals forces, the present methodology yields results that are consistent with the previous studies, which further validates the present methodology. Different from these previous studies, the present methodology is able to probe a much wider parameter space.

The contributions of the present study are twofold. First, a general methodology is proposed through which one can deduce a rheological model for granular materials with various properties. To illustrate its viability, the methodology is applied in the study of monodisperse non-cohesive particles and particles with interparticle van der Waals forces, and kinetic-theory based model is verified and augmented. This general methodology can be readily applied to other systems where particles can be polydisperse and particle-particle interactions can be complex, and the rheological model can be formulated based on other models.

Second, modified kinetic-theory-based models are proposed for non-cohesive and cohesive particles. The model is summarized in table 4.2. It should be noted the model parameters are based on simulations performed here with particles with sliding friction coefficient $\mu_p = 0.5$ and restitution coefficient $e_p = 0.9$, which are typical values found in literature. For other values, it is expected that some model parameters need to be slightly adjusted. For example,
it is known that the jamming volume fraction $\phi_c$ would decrease with increasing $\mu_p$ [52]. Compared with prior models proposed based on simulations, the present model accounts for the effects of interstitial fluid and compaction/dilation, and covers a wide range of solid volume fractions. Compared with prior models proposed through derivations, the present model avoids the assumptions required in the derivations, and offers flexibility where a user can propose one’s own models for the particular systems of interest.

In future studies, it is planned to utilize this methodology to propose models for other systems to demonstrate the robustness of this approach. Furthermore, the model developed here is planned to be implemented in CFD solver to assess its performance. Finally, it is planned to coarsen the stress results to obtain a mesoscale stress model [32, 33, 35, 38].
Chapter 5

Neural networks for drag modeling

Overview of the chapter

We propose models for the filtered drag based on results from CFD-DEM simulations of both non-cohesive and cohesive particle fluidization in a fully periodic domain. We apply neural networks in modeling which take advantage of the abundance of data available from simulations, and demonstrate that they provide a substantial boost to model performance compared with traditional approaches. Specifically, we show that the proposed neural network model, without retraining, can work reasonably well for particles with any particle size, cohesion level, and filter size. As part of the study, we also show that the information from neighboring cells provides an improvement in the modeling performance. Finally, we demonstrate that one can obtain physical insights from neural networks based on analyzing the feature importance in the trained model.

1The work in this chapter is based on a manuscript under preparation: Y. Gu, J. Kolehmainen, A. Ozel, and S. Sundaresan. Neural networks for drag modeling in fluidization.
5.1 Introduction

Neural networks [189] are ubiquitous in our daily life, often without us knowing it. When you purchase products, search for information, or simply view an advertisement on the internet, you are likely interacting with a model based on neural networks. Its revival as the preferred data-driven method is not only driven by external factors such as an abundance of data and increased computational power, but also the recent breakthroughs in the field, specifically on how to effectively train them (e.g. [190–193]). Neural networks prove to be transformative in many fields, and they have been demonstrated to beat other machine learning techniques for diverse scientific applications, such as predicting the activity of potential drug molecules [194] and analyzing particle accelerator data [195], to name a few.

Neural networks excel in applications where there is an abundance of data, and human knowledge of the problem is lacking. Instead of human handpicking model formulations based on physical intuition through a trial and error process, neural networks automatically discover the optimal representations of raw data for the particular task. Mostly importantly, unlike the human counterpart, the predicting power of neural networks scales with the amount of data available. These features of neural networks are attractive for multi-scale modeling of fluid flows. In multi-scale modeling of fluid flows, modelers often need to formulate coarse-grained models based on data from direct numerical simulations (DNS). With increased computational power, DNS can generate large amounts of data, which the traditional approaches based on physical intuition cannot take advantage of. For example, in the present study, we have around 2 million data points for each snapshot of the simulation. It is a daunting task already to manually inspect just one of these simulation snapshots to look for patterns to aid the model development. Neural networks provide the tools to allow the modeler to take advantage of these large amount of data. Specifically, neural networks help the modeler to accomplish two tasks. First, neural networks provide an engineering solution for the modeler to develop the best or close to the best model for a given problem. Second,
neural networks can be used by modelers to probe the physics of the system; the modeler can adjust the variables that are fed into the neural networks to investigate the importance of specific variables.

These two advantages of neural networks are both demonstrated in the present study. Specifically, we apply neural networks to multi-scale modeling of gas-particle flows in fluidized beds. It is well known that they manifest inhomogeneous structures over a wide range of length and time scales, which are difficult and expensive to resolve in simulations [35]. Filtered models [30, 32] aim to resolve only the coarse, macro-scale flow structures which are often of most interest for practical applications. The effects of unresolved fine-scale structures are accounted for through closures in terms of filtered variables. For the past decade, several studies have developed these closures based on fine-grid simulations [30–34, 38, 196–198]. It is now known that the filtered drag force can be significantly smaller than that predicted by the original drag force models, and this correction plays the most important role.

These modeling attempts for the filtered drag term fall into two categories. In the first generation, the filtered drag force is expressed as a function of filtered variables within the computational cells [30–33, 197]. In the second generation, additional markers of filtered variables from surrounding cells are used [34, 196, 198]. In this later generation model, how to effectively combine the information from surrounding cells has largely been based on physical intuition. In contrast, neural networks can provide an optimal representation of this information from large amounts of data. In the present study, we run fine-grid simulations, and post-process the results to propose models for the filtered drag force using neural networks. We show that the neural-network based model that uses the information from surrounding cells provides superior predictability performance, as it can work for any particle size, interparticle cohesion, or any filter size without retraining the model. To highlight the importance of using information from surrounding cells, we also build a neural network based on variables within the computation cell, and show that it would result in
poor predicting performance. Lastly, we demonstrate that we can learn the importance of variables fed into the neural network model, and gain a physical understanding of the model.

5.2 Methodology

5.2.1 Multi-Layer Perceptron

Multi-layer perceptron (MLP), which is the most basic type of neural network, is used in the present study. It is loosely based on the anatomy of the brain, as it is composed of densely interconnected computing nodes organized into layers. The connections between nodes of adjacent layers are determined by weights, which specify how much nodes in one layer would contribute to the nodes in the next layer. During training where data is fed into MLP, these weights are optimized to minimize the difference between the model’s output and the actual values.

Two neural network architectures are explored here, as shown in figure 5.1. There are one hidden layer in (a), and 7 hidden layers in (b). In the following, we provide a short discussion on how MLP for these two architectures works. For more information on MLP and neural networks in general, the reader is referred to the textbook by Goodfellow et al. [199]. For a given data set, we have features and target values. For the features, we have a matrix $X$ with dimension of $n_x$ by $m$. Here, $n_x$ is the number of features, and $m$ is the number of data points. For the target, we have a matrix $y$ with dimension of 1 by $m$. Values for each feature in $X$ are first scaled to have a mean of 0 and standard deviation of 1, to facilitate optimization. Feature matrix $X$ is then fed into input layer. From the input layer to the next layer, which is a hidden layer with $n_{h,1}$ neurons, the following calculation is used:

$$A_1 = f(W_1 X + b_1).$$

(5.1)
Here, $A_1$ has a dimension of $n_{h,1}$ by $m$, and is the calculated activations for this first hidden layer. $W_1$ is the weight, and $b_1$ is the bias added. $W_1$ has a dimension of $n_{h,1}$ by $n_x$, and $b_1$ has a dimension of $n_{h,1}$ by $m$ with each row having the same value. $f$ is the activation function that introduces non-linearity into the model. It is an element-wise operation, and Rectified Linear Unit (ReLU) [200] is used:

$$f(z) = \max(0, z).$$

(5.2)

This operation as in equation (5.1) is repeated for each subsequent hidden layer, up till the last hidden layer $L$. In (a), $L = 1$, and in (b) $L = 7$.

From the last hidden layer $L$ to the output layer, the following calculation is used:

$$\hat{y} = W_o A_L + b_o.$$  

(5.3)

$A_0$ becomes $X$ in (a). Here, $\hat{y}$ is the model prediction for the target, and has a dimension of 1 by $m$. $W_o$ and $b_o$ are weight and bias terms for the output layer. $W_o$ has a dimension of 1 by $n_{h,L}$, and $b_o$ has a dimension of 1 by $m$.

To characterize the performance of the model, a loss function based on mean absolute error is computed:

$$L(W_1, \ldots W_L, W_o, b_1, \ldots b_L, b_o) = \frac{1}{m} \sum_{k=1}^{m} |y^{(k)} - \hat{y}^{(k)}|.$$  

(5.4)

During training step, this loss function is minimized through back-propagation [201] using an adaptive moment optimization method (commonly referred as “Adam”) [193]. To reduce overfitting, the early stopping strategy is utilized. Specifically, the loss error on the development data set is monitored, and training is halted once the loss error stops decreasing. We discuss below on how these data sets are constructed and chosen.
Figure 5.1: Two neural network architectures used in the study.

5.2.2 Data sets

The same simulation results as in Chapter 4 are analyzed here; we performed CFD-DEM simulations in a periodic domain. Correction to the drag force needed for coarse-grid simulations was computed by filtering the results from these simulations as shown below.

The macroscopic quantities are filtered using various filter sizes $\Delta_f$ around each computational node. The filtered solid volume fraction is computed by

\[
\overline{\phi}(x, t) = \int \int \int \phi(r, t) G(r - x) dr
\]  

(5.5)

where $\phi$ is the solid volume fraction of the local cell, and $G(r - x)$ is a weight function which satisfies $\int \int G(r) dr = 1$. The box filter kernel employed in all the results presented here is given by

\[
G(r - x) = \begin{cases} 
\frac{1}{\Delta_f}, & \text{if } |r - x| \leq \frac{\Delta_f}{2} \\
0, & \text{otherwise.}
\end{cases}
\]  

(5.6)
Similarly, the filtered gas velocity is defined as

$$
\tilde{u}_g(x, t) = \frac{1}{(1 - \phi)} \int \int \int G(r - x)(1 - \phi(r, t)) u_g(r, t) dr,
$$

(5.7)

where \( u_g(r, t) \) is the gas velocity for the local cell. For the particle phase, we first compute the Eulerian solid velocity \( u_s(r, t) \) by mapping the particle velocity \( v(x, t) \) to the cell centers. Then, we compute the filtered solid velocity by

$$
\tilde{u}_s(x, t) = \frac{1}{\phi} \int \int \int G(r - x) \phi(r, t) u_s(r, t) dr
$$

(5.8)

filtered slip velocity by

$$
\tilde{u}_{slip}(x, t) = \tilde{u}_g(x, t) - \tilde{u}_s(x, t),
$$

(5.9)

and the filtered drag coefficient as:

$$
\overline{\beta}_i = \frac{\beta_i (u_{g,i} - u_{s,i})}{(\tilde{u}_{g,i} - \tilde{u}_{s,i})}
$$

(5.10)

where \( \beta_i \) is the “microscopic” drag coefficient (namely, Wen and Yu [51] drag law used in our simulations). Here, the subscript \( i \) denotes the three directions. We focus on its vertical direction here, as it is known to be the most important for general fluidization problems.

Therefore, the target for the data set is chosen to be the drag ratio \( \alpha = \overline{\beta}_{vertical}/\beta_{vertical} \). Two groups of features are used for the data set. The dimensionless filter size, more precisely, its inverse \( d_p/\Delta_f \) is used in both groups. In the first group, only the local information is used. They are the filtered primary variables within the filtered cell, namely, filtered solid volume fraction \( \overline{\phi} \), and filtered slip velocity \( \tilde{u}_{slip} \) in each of the three directions. Thus, the first group has 5 features. In the second group, additional information that is contained in the surrounding 26 cells is used. Thus, we have 109 features: dimensionless filter size \( d_p/\Delta_f \),

151
Table 5.1: Pearson correlation coefficient between values from model predictions \( \hat{y} \) and actual values \( y \)

<table>
<thead>
<tr>
<th>Particle Diameter ( d_p ) (( \mu m ))</th>
<th>Filter size ( \Delta f/d_p )</th>
<th>Including surrounding cells; 1 hidden layer</th>
<th>Including surrounding cells; 7 hidden layers</th>
<th>Local cell only; 1 hidden layer</th>
</tr>
</thead>
<tbody>
<tr>
<td>75</td>
<td>27</td>
<td>0.67</td>
<td>0.66</td>
<td>0.28</td>
</tr>
<tr>
<td>150</td>
<td>27</td>
<td>0.60</td>
<td>0.61</td>
<td>0.13</td>
</tr>
<tr>
<td>300</td>
<td>27</td>
<td>0.69</td>
<td>0.69</td>
<td>0.25</td>
</tr>
<tr>
<td>75 (cohesion)</td>
<td>39</td>
<td>0.60</td>
<td>0.49</td>
<td>0.24</td>
</tr>
<tr>
<td>75</td>
<td>39</td>
<td>0.69</td>
<td>0.56</td>
<td>0.24</td>
</tr>
</tbody>
</table>

filtered solid volume fraction \( \bar{\phi} \) for the 27 cells, and filtered slip velocity \( \tilde{u}_{slip} \) in each of the three directions for the 27 cells.

To prevent neural network model from overfitting, it is crucial to have separate training, validation, and testing data sets. Training set is fed into neural networks to optimize the weights, and validation set is used to tune hyper-parameters of the neural networks (including early stopping as discussed before). Testing set is finally used to evaluate the model. To ensure that training, validation, and testing data sets are distinct, different time steps are chosen between the sets. For training set, we use 6 snapshots (around 12 million data points in total): (1-2) \( d_p = 75 \mu m, \Delta f = 27d_p \) at two different time steps; (3) \( d_p = 75 \mu m, \Delta f = 15d_p \); (4) \( d_p = 75 \mu m, \Delta f = 33d_p \); (5) \( d_p = 150 \mu m, \Delta f = 27d_p \); (6) \( d_p = 300 \mu m, \Delta f = 27d_p \).

### 5.3 Results

To evaluate the performance of the trained neural networks, Pearson correlation coefficient between exact filtered drag ratio and the predicted value is computed for the testing
Figure 5.2: Parity plot for two cases. In (a), information from surrounding cells is included; (b) information from the local cell only is used. One hidden layer is used for both cases. $d_p = 75\mu m$; $\Delta f/d_p = 27$.

data set. The Pearson correlation coefficient is defined as

$$r(\hat{y}; y) = \frac{\sum_{k=1}^{m}(\hat{y}^{(k)} - \bar{\hat{y}})(y^{(k)} - \bar{y})}{\sqrt{\sum_{k=1}^{m}(\hat{y}^{(k)} - \bar{\hat{y}})^2} \sqrt{\sum_{k=1}^{m}(y^{(k)} - \bar{y})^2}}$$

(5.11)

where the bar denotes the average.

To visualize the model performance, we also plot the probability density function of relative error $e_i$:

$$e_i(\hat{y}; y) = \frac{\hat{y}^{(i)} - y^{(i)}}{y^{(i)}}.$$

(5.12)

The results on Pearson correlation coefficients are shown in Table 5.1; we also show a parity plot in Figure 5.2, and a plot on relative error in Figure 5.3. As seen in Table 5.1, the trained neural networks using only information from the local cell has a low Pearson correlation coefficient of around 0.2; this poor performance is further confirmed by the parity plot in
Figure 5.3: Probability density function of relative error. $d_p = 75\mu m$; $\Delta f/d_p = 27$; information from surrounding cells is included; 1 hidden layer is used.

Figure 5.2(b). A previous model based on information from the local cell [33] was indeed found [202] to have a Pearson correlation coefficient of about 0.1.

For the same data set as studied here, Ozel et al. [202] proposed a model that uses information from surrounding cells via a scale-similar approach [32, 196], and yields a Pearson correlation coefficient of slightly larger than 0.2; the study restricted choice to specific functional forms. In contrast, neural networks approach circumvents the need for pre-specifying functional forms. With neighboring cell information, it yields a Pearson correlation coefficient of over 0.6 (see Table 5.1), even when the test data sets include several particle sizes and cohesion levels; the parity plot for this case is shown in Figure 5.2(a) and its plot on relative error in Figure 5.3.

It is remarkable that this model without retraining works for different particle sizes and both non-cohesive and cohesive particles, without having $d_p$ or cohesion level as an input feature (Table 5.1). This result suggests that this neural network can work with any system, without even knowing the particle properties such as particle size and cohesion level. Further, even though neural networks have only seen data during training for the cases with $\Delta f = 15d_p$, $\Delta f = 27d_p$, $\Delta f = 33d_p$, it learns to extrapolate to the case of $\Delta f = 39d_p$. This result suggests that this neural network can work for any filter size.
As shown in the table, as the hidden layer is increased to 7, there is no improvement in the model performance, which indicates that 1 hidden layer is sufficient to capture the complexity of the system.

While it is difficult to extract feature importance from neural network, the following approach, even though not perfect, is used here to obtain some clues as to what the neural network is doing behind the scene. Specifically, we perturb each variable by adding a small number to it while keeping other variables constant. We then rank the variable based on the change to the prediction. The results are shown here, where we rank the 109 variables (from the most important):

0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 1, 0, 1, 0, 0, 1, 0, 0, 3, 1, 0, 0, 3, 1, 2, 1, 2, 0, 1, 1, 3, 1, 1, 2, 3, 2, 3, 1, 0, 1, 1, 0, 3, 1, 3, 2, 1, 4, 1, 2, 3, 1, 2, 1, 1, 3, 3, 1, 0, 2, 3, 3, 1, 2, 0, 1, 2, 0, 2, 0, 3, 1, 3, 2, 2, 3, 2, 3, 2, 3, 2, 3, 2, 2, 2, 2, 2, 3, 2, 0, 3, 3, 3, 1, 3, 2, 2, 2, 3, 2, 0, 3, 2, 2.

Here, 0 represents the vertical filtered slip velocity, 2 and 3 represent the horizontal filtered slip velocity, 1 represents the filtered solid volume fraction, and 4 represents the filter size. We can see that filtered slip velocities at vertical direction (0) are shown to be most important, followed by filtered solid volume fraction (1). Filter size is ranked in the middle, and filtered slip velocities at horizontal directions are ranked the last. This ranking of variable importance is consistent with previous research (although the fact that filtered solid volume fraction is ranked lower than vertical filtered slip velocity is a little surprising). However, this neural network model is able to account for variables from neighboring cells in a more sophisticated manner than previous models (such as the scale-similar based model discussed before), which results in a huge lift in its performance.

Following this analysis, we investigate the changes to the model performance if we only include a subset of the features. Specifically, we consider three different subsets of the 109
Figure 5.4: Probability density function of relative error for different sets of features. Following the sequence in the legend, in the first one (solid line), the original full set of 109 features is used. In the second one (dashed line), in addition to the filter size, we only keep the filtered solid volume fractions and vertical filtered slip velocities, resulting in 55 features. In the third one (line with circles), in addition to the filter size, we only keep the filtered solid volume fractions for all the 27 cells and the vertical filtered slip velocity for the local cell, resulting in 29 features. In the last one (line with triangles), in addition to the filter size, we only keep the vertical filtered slip velocities for all the 27 cells and the filtered solid volume fraction for the local cell, also resulting in 29 features. $d_p = 75\mu m$; $\Delta_f/d_p = 27$; 1 hidden layer is used in the neural network.
features which account for the information from the surrounding 26 cells. In the first subset, in addition to the filter size, we only keep the filtered solid volume fractions and vertical filtered slip velocities, resulting in 55 features. In the second subset, in addition to the filter size, we only keep the filtered solid volume fractions for all the 27 cells and the vertical filtered slip velocity for the local cell, resulting in 29 features. In the third subset, in addition to the filter size, we only keep the vertical filtered slip velocities for all the 27 cells and the filtered solid volume fraction for the local cell, also resulting in 29 features. Plots on relative errors of the test case of $d_p = 75\mu m$ and $\Delta f/d_p = 27$ are shown in Figure 5.4 for these three subsets compared with the original full set. We also evaluate the Pearson correlation coefficients; compared with the original set that has a value of 0.67, the first subset has 0.62, the second one 0.55, and the third one 0.54. Therefore, compared with the original full set, the first subset has similar performance, but the second and third subsets have substantial drops in performance. These results indicate that (1) the horizontal filtered slip velocities are not essential in predicting filtered drag (2) both vertical filtered slip velocities and filtered solid volume fractions from the surrounding cells are important in describing the filtered drag. These conclusions are consistent with the previous analysis based on perturbations on individual features, and imply the need to include both filtered slip velocities and filtered solid volume fractions from surrounding cells in building physics-based constitutive models for drag.

5.4 Conclusions

In this study, based on results from CFD-DEM simulations, we apply neural networks to propose a filtered drag model that is shown to possess superior modeling ability over previous approaches. Here are the highlights of the study:
• The proposed neural network model, without retraining, can work reasonably well for particles with any particle size, cohesion level, and filter size.

• Through neural network modeling, we show that the information from neighboring cells provides an improvement in the modeling performance. Physically, this result implies that the gradients in primary filtered variables could be important and that future constitutive models should include them.

• We show that one can gain knowledge on the relative importance of various variables from neural network models.
Chapter 6

Summary and suggestions for future work

6.1 Summary

This thesis aims to develop a general approach through which one can develop constitutive models that are required to simulate industrial-scale fluidized beds of particles with any given property. We use the van der Waals force of interaction as an example, show that one can start with a small-scale detailed DEM and CFD-DEM simulations where one can directly specify particle properties, progressively coarse-grain the simulation results, and finally obtain constitutive models of drag and particle phase stress that are required for filtered TFM/MP-PIC. One can then run filtered TFM/MP-PIC with these closures that are “tailor-made” for these particle properties.

To develop these required constitutive models for drag and particle phase stress, in Chapter 2 we focus on developing a micro-scale particle phase stress model for particles with cohesion or particle size distributions at dense regime using DEM-based simple shear simulations.
Specifically, we study the effects of both van der Waals force and particle size distribution on particle phase stress. We find that the van der Waals force gives rise to a new flow regime where stress is shear rate independent. Introducing particle size distribution increases the jamming solid volume fraction in a systematic way that can be related to the distribution of particle size. Therefore, we are able to propose a stress model that can describe dense flow for cohesive and polydisperse granular materials.

In Chapter 3, we develop and validate the CFD-DEM approach that appropriately accounts for interparticle cohesion. In developing the CFD-DEM simulation approach, we propose a modified cohesion model to be used in the simulation. To speed up simulations, many studies in literature adopt small particle spring constants to allow for larger time steps. We show that this practice would yield unphysical results for cohesive particles. A modified cohesion model is then proposed so that the simulation results are insensitive to particle spring constant. We then apply this modified cohesion model and the CFD-DEM approach to probe the effects of fines on fluidization. Previous experiments have found that adding fines to fluidization would reduce bubble sizes. However, the mechanism is little understood. We show that the present CFD-DEM approach with the newly developed modified cohesion model can qualitatively capture this behavior, which then allows us to probe the underlying physics. Thus, this study not only supports the validity of the modified cohesion model and CFD-DEM approach, but also helps elucidate the mechanism behind the bubble size reduction with fines. Specifically, the beneficial effect of fines takes place through cohesive interaction between the fines and the larger particles.

After developing and validating the CFD-DEM approach that appropriately accounts for interparticle cohesion in Chapter 3, we apply the approach to simulate systems in a periodic domain in Chapter 4. We develop a novel methodology through which one can propose micro-scale stress models for both non-cohesive and cohesive particles by analyzing results from these simulations. Compared with the stress model in Chapter 2, the model developed
in Chapter 4 has two advantages. First, it accounts for the effects of interstitial fluids. Second, it covers a wider range of parameter space. We first validate this methodology using non-cohesive particles, and show that it yields models that are consistent with the analytically derived kinetic theory. We then propose the stress models for cohesive particles. Thus, we are able to propose a stress model for both non-cohesive and cohesive particles that accounts for the effects from interstitial fluids and covers a wide range of flow regimes.

In Chapter 5, we use the same CFD-DEM simulation results as in Chapter 4, and propose filtered drag models for both cohesive and non-cohesive particles. We apply neural networks in modeling, and demonstrate that they provide a substantial boost to the model performance compared with previous traditional approaches. Specifically, we show that the proposed neural network model, without retraining, can work reasonably well for particles with any particle size, cohesion level, and filter size.

6.2 Suggestions for future work

In Chapter 5, we show that neural networks can model filtered drag better than traditional approaches. The modeling ability of neural network would even become stronger in the coming years, as the computational power improves, algorithm is further optimized, and more advances in the field of neural networks are made. In light of these factors, there is much evidence to believe that neural network will play an indispensable role in both improving other modeling ability and our physical understanding of fluidization.

This thesis is one of the first studies to apply neural networks to examine coarse-grained closures for fluidization. Here, we offer several suggestions for future work on this topic.

First, one can apply neural networks to model other closures such as those that describe the filtered interphase heat/mass transfer and filtered scalar diffusion which are needed to
model scaler transport [203], as well as the particle phase stress. It is envisioned that we can apply multi-task learning in neural networks, in which we have only one neural network that outputs all the values for closures including filtered drag, particle phase stress, etc. This approach could be feasible because that all the intermediate hidden layers learn the physics that can be used for different tasks.

Second, one can utilize more complex neural network architectures to further improve the predicative power of the model. The neural network in this thesis is Multilayer Perceptron (MLP), which is the most basic class of neural networks. Fluidization problems span in time and space, and there are many neural network classes that can take advantage of the temporal and spacial features of this problem. For example, one can envision having a model for filtered drag that is a function of not only the adjacent cells, but the next layer (or even more layers) of cells too. To train this neural network properly, Convolutional Neural Network (CNN) [204] would be a more suitable choice. In another example, one can envision having a model for filtered drag that is a function of not only the variables in the present time, but also those in the past. Recurrent Neural Network (RNN) [205], especially Long-Short Term Memory (LSTM) [206], would be a great candidate for this task.

Third, one can look into how to best interpret the trained neural network to help discover the underlying physics. This objective on interpreting neural network is an active research area in the machine learning community. To find the importance of features, one of the most reliable approach is wrapper model feature selection. In this approach, one “wraps” around the learning algorithm (neural network here), and uses a subset of the feature to evaluate the model performance. The shortcoming of this approach is that this approach would be computationally expensive if one has many features and/or each training is computationally expensive. The perturbation approach introduced in Chapter 5 is much less computationally intensive. However, the perturbation is only applied on one combination of variables. Therefore, the analysis is restricted. Another existing approach is to use a different ma-
chine learning method that can output the feature importance. The most commonly applied method for this purpose is random forests [207] which is an ensemble learning method based on decision trees. Random forests in most cases can achieve similar modeling accuracy as neural network, but can also provide information on feature importance. One then can build a model based on random forests in addition to the one based on neural networks for the same problem, and gain the feature importance. The disadvantage of this method is that, enabling random forests to have the similar performance as neural networks would call for computationally expensive training.

It should be emphasized that the application of neural networks for modeling discussed here is not restricted to fluidization problems, but for fluid dynamics in general. As pointed out by a recent paper [208], neural networks would play a “critically enabling role in the future of modeling complex flows”. We cannot wait to see how transformative it can be in the coming years.
Bibliography


