Granular materials are mixtures of discrete, macroscopic particles. They are ubiquitous in nature as well as in everyday life – in forms such as sand, gravel, pharmaceutical pills, food grains, and industrial powders. However, certain mechanical behaviors of these materials are still beyond the community’s understanding, including flow and size-segregation phenomenon. Compared to other common engineering materials such as elastic solids and viscous fluids, modeling of granular flow has remained a persistent challenge, especially from a continuum perspective. This thesis addresses several problems related to the continuum modeling of dense granular materials:

- Dense granular heap flows (e.g., avalanches and landslides in nature) consist of a rapid flow regime localized near the free surface and a creeping flow region deep beneath the surface. We apply a scale-dependent continuum approach – the nonlocal granular fluidity model – to a representative steady, dense granular heap flow setup and successfully capture the salient features of both regions, which existing continuum models have not been able to simultaneously predict.

- The flow threshold of dense granular materials exhibits a size effect that cannot be captured by conventional local, stress-based criteria. Using two-dimensional discrete element method calculations, we explore the configurational generality of the size-dependence of the flow threshold – i.e., additional strengthening with smaller system size – and show that the nonlocal granular fluidity model is capable of quantitatively capturing this effect.

- Dense granular systems consisting of particles of disparate sizes segregate based on size during flow, resulting in complex, coupled segregation and flow patterns. We study the two driving forces of size-segregation – pressure-gradients and shear-strain-rate-gradients – in dense flows of bidisperse disks and show that both the flow fields and the segregation dynamics may be simultaneously captured by coupling a segregation model with the nonlocal granular fluidity model.
Continuum Modeling of Flow and Size-Segregation in Dense Granular Materials

by
Daren Liu
B. S., University of Science and Technology of China, 2013
Sc. M., Brown University, 2015

A dissertation submitted in partial fulfillment of the requirements for the Degree of Doctor of Philosophy in School of Engineering at Brown University

Providence, Rhode Island
May 2019
© Copyright 2019 by Daren Liu
This dissertation by Daren Liu is accepted in its present form by
the School of Engineering as satisfying the dissertation requirement
for the degree of Doctor of Philosophy.

Date ___________  ________________________________

David Henann, Ph.D., Advisor

Recommended to the Graduate Council

Date ___________  ________________________________

Kenneth Kamrin, Ph.D., Reader

Date ___________  ________________________________

Kyung-Suk Kim, Ph.D., Reader

Date ___________  ________________________________

Tom Powers, Ph.D., Reader

Approved by the Graduate Council

Date ___________  ________________________________

Andrew G. Campbell, Ph.D.
Dean of the Graduate School

iii
Curriculum Vitæ

Daren Liu was born on January 16th, 1992 in Ji’an, Jiangxi Province of southeast China. He started his undergraduate study at the University of Science and Technology of China in 2009, and received a Bachelor of Science degree in Theoretical and Applied Mechanics in 2013. In the fall of that year, he started graduate work in the Mechanics of Solids program at Brown University, and attained a Master of Science degree in Solid Mechanics in 2015.

Refereed Journal Publications

(1 = These authors contributed equally.)


Conference Proceedings

(1 = talk, 2 = poster)


“Modeling shear-rate-gradient-driven size-segregation in dense, bidisperse granular flows”. 16th Annual Northeastern Granular Materials Workshop, Yale University, Jun. 8th, 2018.1
“Modeling shear-rate-gradient-driven size-segregation in dense, bidisperse granular flows down a vertical chute”. APS March Meeting 2018, Los Angeles, California, Mar. 5th - 9th, 2018.¹


**Teaching Experience at Brown**

**Undergraduate**

Advanced Mechanics of Solids, TA (Fall ’14)

**High School**

Introduction to Engineering and Design, Instructor (Summer ’18)
Acknowledgements

“The academic journey is as much about finding truth in books and experiments as it is about finding truth in yourself.” — “Piled Higher and Deeper”.

My own graduate journey would certainly not be completed without standing on shoulders of mountains of people. Lessons, meetings, experiences, even brief encounters or conversations that sometimes seem small, shape me into who I am today.

I am so very proud and fortunate to be the first student of my advisor/role model, Prof. David Henann, a true mentor and dedicated scholar. I see from you the pure love and passion towards science and research. Over the years I have been privileged to have the freedom to explore, to experience, and your constant and consistent kindness, support, patience, positiveness and respect have made this journey quite enjoyable and memorable. I don’t know how many times I walked in your office with unpleasant results in frustration, while you would always respond with smile, patiently dive into the details with me, and use your insights to point me in the right direction. I truly appreciate these positive impacts you’ve had on me.

I would like to express my gratitude towards my thesis committee for willingly taking the time to read my thesis and provide valuable feedback. Prof. Kyung-Suk Kim and Prof. Tom Powers, I also enjoyed your classes. Prof. Ken Kamrin, this thesis would not be possible without you paving the fundamentals and your continuous inputs. A bunch of thanks also goes to Prof. Huajian Gao, Prof. Haneesh Kesari, Prof. Allan Bower, among other faculty and staff members in the School of Engineering.

With five years and a half spent here, the distinguished Brown University with its plentiful resources and openness, and the historic Providence with its bitter New England winter,
have in a sense become my second home. To be surrounded by so many smart and interest-
ing people from diverse backgrounds is most fantastic. I am happy to see the Arnold 322
family growing over the years: Shihong, Yuhao, Mike, Xiuqi, Natassa and Harkirat. I will
cherish our exhilarating office environment, and I wish we could had done those dinner and
movie nights more often. To my peer students in Solids and our remarkable Engineering
community, many of you assisted me in various occasions. I know I would definitely miss
someone if I start listing names, so I will just say I am so much obliged to you for all the
help and support that carried me along the way. Thank you. You know who you are.

To the many wonderful friends, you kept reminding me to not always bury my face into
papers and codes and instead take a break once in a while and live a balanced life. Special
thanks to Chao, Xizheng, Zhiyu, Li, An, for the long-lasting friendship. Zheng, Wenzhe,
Boda, Xi, Yinsui, Shihong, Siyi, Guangyao, Zhi, our trips to Britain, Italy, Turkey, Mexico,
Alaska really opened up my eyes. Connie, thank you for praying for me and pushing me to
dream big when I lacked will. To the Brown Chinese Dragon Soccer Team and generations
of intramural teammates, it is my pleasure to have played with you. And to my remote
friends in China, thanks for the wishes from the other side of the Earth.

Most importantly, none of this would be possible if not for the love from my parents,
Yicheng and Xiaoqing. I can only imagine how you hid your feelings and sacrificed your
need of companion from your only child in lunar new years seeing other families in reunion.
Thank you mom and dad for letting me do what I love and always cheering for me. I love
you.
DEDICATED TO MY TEACHERS, MENTORS, MY DEAR PARENTS, AND ALL OF THOSE WHO LOVE AND SUPPORT ME AS ALWAYS.
## Contents

**List of Tables** xiii

**List of Figures** xv

### 1 Introduction 1

1.1 Background on dense granular materials and continuum modeling . . . . . 1  
1.2 Thesis contributions . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 3  
  1.2.1 The nonlocal granular fluidity model on steady, dense heap flows . . 4  
  1.2.2 Size-dependent flow threshold of dense granular materials . . . . . 4  
  1.2.3 Modeling size-segregation in dense, bidisperse granular flows . . . . 5  
1.3 Thesis outline . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 5

### 2 Nonlocal continuum modeling of steady, dense granular heap flows 7

2.1 Introduction . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 7  
2.2 The nonlocal granular fluidity model . . . . . . . . . . . . . . . . . . . . . 11  
2.3 Numerical simulations of dense, steady granular heap flow . . . . . . . . 16  
  2.3.1 Flow configuration . . . . . . . . . . . . . . . . . . . . . . . . . . . 17  
  2.3.2 Flow fields . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 20  
  2.3.3 Volume flow-rate and maximum velocity . . . . . . . . . . . . . . . 23  
  2.3.4 Two length scales . . . . . . . . . . . . . . . . . . . . . . . . . . . 25  
2.4 Concluding remarks . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 26

### 3 Size-dependence of the flow threshold in dense granular materials 29

3.1 Introduction . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 29  
3.2 Discrete-element method simulations . . . . . . . . . . . . . . . . . . . . . 32  
  3.2.1 Simulated granular system . . . . . . . . . . . . . . . . . . . . . . 32  
  3.2.2 Planar shear flow . . . . . . . . . . . . . . . . . . . . . . . . . . . 34  
3.3 Granular rheology and the flow threshold . . . . . . . . . . . . . . . . . . . 36  
3.4 Flow threshold in other configurations . . . . . . . . . . . . . . . . . . . . 42  
  3.4.1 Planar shear flow with gravity . . . . . . . . . . . . . . . . . . . . 43  
  3.4.2 Annular shear flow . . . . . . . . . . . . . . . . . . . . . . . . . . 48  
  3.4.3 Vertical chute flow . . . . . . . . . . . . . . . . . . . . . . . . . . 52  
3.5 Concluding remarks . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 56

### 4 Modeling shear-rate-gradient-driven and pressure-gradient-driven size-segregation in dense, bidisperse granular flows 59

4.1 Introduction . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 59  
4.2 Continuum framework . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 63
List of Tables

4.1 Summary of the quantities introduced to describe dense, bidisperse granular mixtures ........................................... 64
List of Figures

1.1 Examples of granular materials and common applications .......................... 2

2.1 Heap flow schematic and computational domain ................................. 18
2.2 Flow fields in a narrow channel of width $W/d = 19$ for steady, dense granular heap flow .......................................................... 20
2.3 Flow fields in a wide channel of width $W/d = 142$ for steady, dense granular heap flow .......................................................... 23
2.4 Relationships between free surface inclination angle, maximum velocity, and volume flow-rate in steady, dense granular heap flow ......................... 24
2.5 Calculated dependence of the size of the flowing zone and the creeping zone decay length on the volume flow-rate in steady, dense granular heap flow ......................................................... 25

3.1 Configuration and flow threshold locus for inclined plane flow .................. 30
3.2 Configuration for planar shear flow and calculated local inertial rheology .... 34
3.3 Configuration for planar shear flow with gravity, dependence of the stress ratio at the wall on wall speed, flow threshold locus, and steady velocity fields in the quasi-static regime ................................................. 43
3.4 Configuration for annular shear flow, dependence of the stress ratio at the wall on wall speed, flow threshold locus, and steady velocity fields in the quasi-static regime ................................................. 49
3.5 Configuration and flow threshold locus for vertical chute flow .................. 52
3.6 Comparison of the analytical flow thresholds predicted by the NGF model for inclined plane flow, planar shear flow with gravity, annular shear flow, and vertical chute flow ......................................................... 57

4.1 A representative sub-domain of a dense, bidisperse granular system consisting of two-dimensional disks ......................................................... 63
4.2 Configuration for planar shear flow and calculated local inertial rheology for dense, bidisperse granular systems ................................................. 66
4.3 Binary diffusion coefficient versus $γd^2$ in DEM simulations of homogeneous, steady planar shearing of dense, bidisperse granular systems ............. 70
4.4 DEM simulation of bidisperse vertical chute flow .................................. 72
4.5 Collapse of diffusion flux versus segregation flux in quasi-steady vertical chute flow of bidisperse disks ......................................................... 74
4.6 DEM simulation of bidisperse annular shear flow .................................. 77
4.7 Collapse of diffusion flux versus segregation flux in quasi-steady annular shear flow of bidisperse disks ......................................................... 79
<table>
<thead>
<tr>
<th>Section</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.8</td>
<td>Comparisons of the coupled continuum model predictions with corresponding DEM simulation results during transient flow and for five vertical chute flow test cases.</td>
</tr>
<tr>
<td>4.9</td>
<td>Comparisons of the coupled continuum model predictions with corresponding DEM simulation results during transient flow and for five annular shear flow test cases.</td>
</tr>
<tr>
<td>4.10</td>
<td>DEM simulation of bidisperse inclined plane flow.</td>
</tr>
<tr>
<td>4.11</td>
<td>Collapse of the difference between diffusion flux and shear-rate-gradient-driven segregation flux and the pressure-gradient-driven segregation flux in quasi-steady inclined plane flow of bidisperse disks.</td>
</tr>
<tr>
<td>4.12</td>
<td>Comparisons of the coupled continuum model predictions with corresponding DEM simulation results during transient flow and for five inclined plane flow test cases.</td>
</tr>
<tr>
<td>4.13</td>
<td>DEM simulation of bidisperse planar shear flow with gravity.</td>
</tr>
<tr>
<td>4.14</td>
<td>Collapse of the difference between diffusion flux and shear-rate-gradient-driven segregation flux and the pressure-gradient-driven segregation flux in quasi-steady planar shear flow of bidisperse disks with gravity.</td>
</tr>
<tr>
<td>4.15</td>
<td>Comparisons of the coupled continuum model predictions with corresponding DEM simulation results during transient flow and for five planar shear flow with gravity test cases.</td>
</tr>
<tr>
<td>4.16</td>
<td>Collapse of diffusion flux versus fluidity-gradient-driven or granular-temperature-gradient-driven segregation flux in quasi-steady vertical chute flow and annular shear flow of bidisperse disks.</td>
</tr>
<tr>
<td>C.1</td>
<td>DEM simulation of planar shear flow of an initially-segregated bidisperse granular system.</td>
</tr>
</tbody>
</table>
Chapter 1

Introduction

1.1 Background on dense granular materials and continuum modeling

A granular material is a collection of discrete, macroscopic particles. Granular materials are a common class of materials appearing in everyday life as well as playing a vital role in a variety of industries, such as geophysical, pharmaceutical, food processing, and energy, in forms of sand, soil, debris, pills and powders, as well as food grains (illustrated in Fig. 1.1). In fact, granular material is second only to water as the most common industrial material [1].

Due to their ubiquity and broad applications, the flow behavior of granular materials has received much attention from both the scientific and industrial communities. One major focus of the research on granular media is understanding the physics and mechanics behind the many flow behaviors and then formulating models aimed at capturing the salient flow features, which remains a challenge. The lack of predictive models for granular flow is a long-standing and costly problem in engineering design involving granular materials, and the benefits from improved granular flow modeling are abundant. For example, it is estimated that 40% of capacity is wasted due to over-design of equipment and handling
Figure 1.1: Examples of granular materials and common applications: (a) geophysics, (b) pharmaceutical industry, (c) Mars rover “Spirit” in sandy terrain, and (d) food industry.

For a dry granular system, grain-grain interactions (repulsive forces) only occur when in contact, and the evolution of the positions of constituent grains follows Newton’s Law without being affected by thermal fluctuations. From that perspective, one might conclude that the behavior of an assembly of grains is very intuitive and deterministic, and this first impression could lead one to model granular materials using the Discrete Element Method (DEM) [3], which simulates the whole granular system particle-by-particle. Indeed, DEM can serve as a good tool in many situations, but computation time quickly becomes a bottleneck as the system size scales up, making it difficult to handle many real industrial problems involving granular materials. Also, the predictivity of DEM is based on the fidelity of the grain-grain contact model, and it is users’ responsibility to make sure the applied model physically reflects the problem.

On the other hand, continuum models, which treat the granular media as a continuous mass instead of considering discrete particles, are desirable for predicting granular flows – just as for other materials in engineering design – since a continuum approach enables numerical implementation utilizing the finite-element method (FEM), which is speedier...
than DEM. In fact, researchers have been working on obtaining continuum models for the mechanical behavior of granular materials for many years [4–5]. Some models do succeed in predicting certain features but are often only applicable to specific flow conditions. Many complicating factors arise, and an effective general model remains elusive. It turns out, even for the simplest granular system - a collection of dry, hard spheres that are roughly all the same size (monodisperse) - flow in a slightly complicated geometry can be very complex and difficult to predict. For example, the inertial rheology [7–10] is a common and popular continuum model that fully describes a monodisperse granular system in planar shear flow. Nevertheless, issues such as nonlocality and size-effects [11–17] become apparent in other flow conditions.

The situation becomes yet more complex in non-monodisperse granular systems, in which the constituent particles can differ in size, shape, density, or surface properties, leading to segregation based on species during flow and resulting in strikingly complicated segregation patterns [18]. Segregation during flow is a phenomena related to the “Brazil nut effect,” which occurs when a non-monodisperse granular system is subjected to shaking [19–21]. In industry, segregation can be a undesirable effect when uniform blending is a necessary processing step in food, chemical, and pharmaceutical applications. Granular size segregation is also an interested topic in geophysics, such as observations involving sediment transport or landslides, in which larger grains segregate to the top of a flowing granular media and end up doing the most damage.

1.2 Thesis contributions

The overarching motivation of this thesis is to develop a more general and easy-to-use continuum model that can be applied to study the flow of dense, monodisperse granular materials and the size-segregation in dense, bidisperse granular systems. Specific problems addressed are summarized as follows.
1.2.1 The nonlocal granular fluidity model on steady, dense heap flows

Dense granular heap flows are common in nature, such as during avalanches and landslides, as well as in industrial flows [7, 9, 12, 22–26]. In granular heap flows, rapid flow is localized near the free surface with the thickness of the rapidly-flowing layer dependent on the overall flow-rate. In the region deep beneath the surface, exponentially-decaying creeping flow dominates with characteristic decay length depending only on the geometry and not the overall flow-rate. Existing continuum models for dense granular flow based upon local constitutive equations are not able to simultaneously predict both of these experimentally-observed features – failing to even predict the existence of creeping flow beneath the surface. In this work, we apply a scale-dependent continuum approach – the nonlocal granular fluidity (NGF) model [27, 28] – to steady, dense granular flows on a heap between two smooth, frictional side walls. We show that the model captures the salient features of both the flow-rate-dependent, rapidly-flowing surface layer and the flow-rate-independent, slowly-creeping bulk under steady flow conditions.

1.2.2 Size-dependent flow threshold of dense granular materials

The flow threshold in dense granular materials is typically modeled by local, stress-based criteria. However, grain-scale cooperativity leads to size effects that cannot be captured with local conditions. In a widely studied example, flows of thin layers of grains down an inclined surface exhibit a size effect whereby thinner layers require more tilt to flow [11]. In this work, we consider the question of whether the size-dependence of the flow threshold observed in inclined plane flow is configurationally general. Specifically, we consider three different examples of inhomogeneous flow – planar shear flow with gravity, annular shear flow, and vertical chute flow – using two-dimensional discrete-element method (DEM) calculations and show that the flow threshold is indeed size-dependent in these flow configurations, displaying additional strengthening as the system size is reduced. We then show that the nonlocal granular fluidity model is capable of quantitatively capturing
the observed size-dependent strengthening in all three flow configurations.

1.2.3 Modeling size-segregation in dense, bidisperse granular flows

Dense granular systems, consisting of particles of disparate sizes, segregate based on size during flow, resulting in complex, coupled segregation and flow patterns [18]. According to current understanding, there are two driving mechanisms of size-segregation in dense granular flows: (i) pressure-gradient (gravity) and (ii) shear-strain-rate-gradient. The mechanism of shear-rate-gradient-driven segregation has received less attention and, as such, is not as well understood. In this work, we start by studying this segregation mechanism in dense flows of bidisperse disks in two flow configurations that eliminates pressure-gradient-driven segregation – vertical chute flow and annular shear flow. Specifically, we perform two-dimensional discrete element method (DEM) simulations, which inform the development of a continuum constitutive model for the segregation dynamics. Similar processes are then repeated for two more configurations – inclined plane flow and planar shear flow with gravity, in which both mechanisms coexist, thereby arriving at a complete segregation model. Coupling this segregation model with the nonlocal granular fluidity (NGF) model, we show that both the flow field and segregation dynamics may be simultaneously captured, which no existing models have achieved.

1.3 Thesis outline

This thesis is outlined around the above three problems. Chapter 2 demonstrates the necessity of a nonlocal rheology, introduces the nonlocal granular fluidity (NGF) model in detail, and applies it to the problem of heap flows. Another application of the NGF model finds itself in Chapter 3 addressing the problem of the size-dependent flow threshold in dense granular materials. In Chapter 4 we couple the NGF model with a segregation model to fully describe the flow and segregation of dense, bidisperse granular mixtures. We close
in Chapter 5 with the major findings of the entire thesis and future research directions.
Chapter 2

Nonlocal continuum modeling of steady, dense granular heap flows

Note: A version of this chapter is published in the Journal of Fluid Mechanics. Data and figures have been used with all co-authors’ consent.


2.1 Introduction

Dense granular flows display many manifestations of grain-size dependence in which cooperative effects at the microscopic grain-level have an observable effect on the macroscopic flow phenomenology – such as wide shear bands in split-bottom flow [13-16], secondary rheology of intruders [17, 29], and the thickness-dependence of the flow threshold in shallow inclined plane flow [11, 30, 31]. Another class of phenomenology affected by cooperativity is dense granular heap flow, such as the flows that arise during avalanches and landslides, in flows down chutes, or in rotating drums. Dense granular heap flow is notable because both rapid, fluid-like flow and slow, quasi-static flow are evident in a single configuration. Steady flow fields are characterized by a rapidly-flowing layer localized at the
free surface with very slow flow beneath [7, 9] [12] 22-26. The thickness of the rapidly-flowing surface layer is strongly dependent on the overall flow-rate. Due to cooperative effects, the rapid surface flow induces creeping flow beneath [12] The creeping flow decays exponentially with the distance from the free surface. In contrast to the thickness of the surface layer, the characteristic decay length of the creeping flow is independent of the overall flow-rate [25].

Simultaneously capturing both the rapid surface flow and the quasi-static, creeping flow with a continuum model has posed a significant challenge and remains an open research question in granular physics. A well-regarded approach, which serves as our starting point, is the inertial rheology [7-9 32], which may be understood through basic dimensional arguments. Consider a quasi-monodisperse granular system with mean grain diameter, \( d \), and grain material density, \( \rho_s \), subjected to homogeneous planar shear with pressure, \( P \), and shear stress, \( \tau \). The consequent shear strain-rate, \( \dot{\gamma} \), may be non-dimensionalized as \( I = \dot{\gamma} \sqrt{d^2 \rho_s / P} \) – referred to as the inertial number. The inertial number operates as a normalized strain-rate and represents the ratio of the microscopic timescale associated with particle motion, \( \sqrt{d^2 \rho_s / P} \), to the macroscopic timescale of applied deformation, \( 1 / \dot{\gamma} \) [7].

The local inertial rheology – local in the sense that it relates the local stress state to the local state of strain-rate at a point – then asserts that the stress ratio, \( \mu = \tau / P \), and the inertial number, \( I \), are related through a one-to-one constitutive relationship, \( \mu = \mu_{loc}(I) \). A common functional form for the local inertial rheology – appropriate for modeling the rapidly-flowing surface layers described above – was proposed by Jop et al. [9]:

\[
\mu = \mu_{loc}(I) = \mu_s + \frac{\mu_2 - \mu_s}{I_0 / I + 1},
\]

(2.1)

where \( \mu_s = \mu_{loc}(I \rightarrow 0) \) is the static yield value, \( \mu_2 = \mu_{loc}(I \rightarrow \infty) \) is the maximum value

\footnote{Following the terminology of Komatsu et al. [12], we use the term creep to describe very slow, quasi-static flow.}
of $\mu$ asymptotically approached as $I$ increases, and $I_0$ is a dimensionless parameter characterizing the nonlinear, rate-dependent response.

The subsequent work of Jop et al. [10] generalized the local rheology (2.1) to three-dimensional flow settings as follows:

Denote the symmetric strain-rate tensor as $\dot{\gamma}_{ij} = \frac{1}{2}(\partial v_i/\partial x_j + \partial v_j/\partial x_i)$ with $v_i$ the velocity vector and $x_i$ the spatial coordinate. Jop et al. [10] began by assuming that steady, dense flow proceeds at approximately constant volume, so that the strain-rate tensor is deviatoric and $\dot{\gamma}_{kk} = 0$. The equivalent shear strain-rate is then defined as $\dot{\gamma} = (2\dot{\gamma}_{ij}\dot{\gamma}_{ij})^{1/2}$. Next, to generalize the stress-related quantities involved in the inertial rheology (2.1) to three dimensions, denote the symmetric Cauchy stress as $\sigma_{ij} = \sigma_{ji}$, and define the pressure $P = -(1/3)\sigma_{kk}$, the stress deviator $\sigma'_{ij} = \sigma_{ij} + P\delta_{ij}$, the equivalent shear stress $\tau = (\sigma'_{ij}\sigma'_{ij}/2)^{1/2}$, and the stress ratio $\mu = \tau/P$. Jop’s three-dimensional form of the local inertial rheology then takes the following form:

$$\sigma_{ij} = -P\delta_{ij} + 2\mu_{loc}(I)P\frac{\dot{\gamma}_{ij}}{\dot{\gamma}}$$

(2.2)

which assumes that the strain-rate tensor and stress deviator are codirectional. When this constitutive model is combined with the equations of motion, the resulting set of governing equations may be used to obtain predictions of steady, dense granular flow in general, three-dimensional flow configurations and has been applied to a variety of problems, such as heap flows [10 25 32], silo drainage [32–35], granular column collapse [35 36], and projectile impact into dense granular media [37]. In the context of steady, dense granular heap flow, aspects of the rapidly-flowing surface layer may be accurately captured; however, as evidenced by the calculations of Jop et al. [10,25] and Kamrin [32], the model also predicts a static zone beneath the rapidly-flowing surface layer. This is because the constitutive relation (2.2) possesses a yield condition in the form of a Drucker-Prager criterion.

---

2Notation: We use standard component notation, which supposes an underlying set of Cartesian basis vectors \{e_i\}_{i=1,2,3}, and in which the components of vectors, $v$, and tensors, $\sigma$, are denoted by $v_i$ and $\sigma_{ij}$, respectively. The Einstein summation convention is employed, and the Kronecker delta, $\delta_{ij}$, is utilized to denote the components of the identity tensor.
in which flow does not occur for $\mu < \mu_s$. Since $\mu < \mu_s$ in the region deep beneath the free surface in dense granular heap flow, the rheology (2.2) predicts that this region is frozen, contrary to experimental observations of exponentially-decaying creep flow. In addition to dense heap flow, a decaying flow profile is experimentally observed in creeping regions where $\mu < \mu_s$ across a variety of configurations, such as annular shear flow [39–42], planar shear flow with gravity [43], and split-bottom flow [13–16]. When applied to these cases, the inertial rheology (2.2) will continue to predict frozen regions with a sharp flow cutoff occurring where $\mu = \mu_s$. The failure of the local inertial rheology to capture creeping flow when $\mu < \mu_s$ stems from the fact that it does not mathematically account for nonlocal, cooperative effects, which become dominant in this regime.

Motivated by this shortcoming, in recent years, nonlocal continuum constitutive models for dense granular flow have been developed, aimed at accounting for cooperative effects [e.g.,44–54]. While these approaches incorporate nonlocality and some have had success in individual geometries, none have been shown to capture the salient aspects of steady, dense granular heap flow. Recently, Kamrin and Koval [27] proposed a nonlocal continuum model – called the nonlocal granular fluidity (NGF) model – inspired by related modeling work in the emulsion community [55, 56], which is capable of quantitatively describing a diverse set of slow, boundary-driven inhomogeneous flows [27, 28], the secondary rheology of intruders [57], and the size-dependence of the flow threshold in inclined plane flow [58]. The purpose of this chapter is to show that the nonlocal granular fluidity model is capable of capturing steady, dense granular heap flow – in particular, the coexistence of a rapidly-flowing surface layer and a creeping bulk. The chapter is organized as follows. In Section 2.2, we discuss the specifics of the NGF model, and in Section 2.3, we apply the model to steady, dense granular flows on a heap between two smooth, frictional side walls. Specifically, in Section 2.3.2, we compare velocity fields predicted by the model with experimentally-measured flow fields from the literature for glass beads [24, 25]. Importantly, the material parameters appearing in the NGF model have previously
been determined for glass beads [9, 28, 59], allowing the NGF model to be applied without parameter adjustment. Then, in Section 2.3.3, we examine the relationships between total flow-rate, maximum velocity, and surface inclination angle, and in Section 2.3.4, we explore the length scales that characterize the coexistent rapidly-flowing and creeping zones. Throughout, our results demonstrate a level of agreement between model predictions and experiments that has not been previously reported. We close with discussion and concluding remarks in Section 2.4.

2.2 The nonlocal granular fluidity model

In this section, we summarize the nonlocal granular fluidity (NGF) model for dense, steady granular flow [see 27, 28, 57, 58, 60]. Similar to the local inertial rheology, the NGF model is valid for granular systems consisting of grains that are (i) spherical, (ii) quasi-monodisperse with constant mean grain diameter \( d \), and (iii) stiff and is intended for steady, well-developed flow conditions. The model consists of three main ingredients: (i) a state parameter, called the granular fluidity, (ii) the flow rule, and (iii) the nonlocal rheology, described in detail below.

1. **Granular fluidity**: Central to the model is the granular fluidity field – a positive, scalar state variable, denoted as \( g \). This state variable is kinematic in nature and characterizes microscopic fluctuations in a flowing granular media. More precisely, Zhang and Kamrin [64] and Bhateja and Khakhar [65] have established that the granular fluidity has a kinematic definition that holds across a variety of inhomogeneous flow configurations for both two- and three-dimensional dense granular systems and is given through the relation 
\[
    g = (\delta v/d)F(\phi),
\]
where \( \delta v \) is the velocity fluctuation, \( \phi \) is the solid volume fraction, \( d \) is the grain size, and \( F(\phi) \) is a function of only \( \phi \).

\(^{1}\)Incorporating particle stiffness into granular rheology is an open research problem. For recent progress on this point, see the works of Campbell [61], Singh et al. [62], and Roy et al. [63].
2. **Flow rule**: For the case of homogeneous planar shear, the granular fluidity relates the stress ratio, \( \mu = \tau / P \), to the consequent shear strain-rate, \( \dot{\gamma} \), through the following constitutive relation:

\[
\dot{\gamma} = g \mu. \tag{2.3}
\]

This one-dimensional version of the flow rule may be generalized to three dimensions following a procedure analogous to that used by Jop et al. [10] to generalize the inertial rheology, discussed in Section 2.1. We define the strain-rate tensor as

\[
\dot{\gamma}_{ij} = (\partial v_i / \partial x_j + \partial v_j / \partial x_i) / 2 - \text{where } v_i \text{ is the velocity field and } x_i \text{ is the spatial coordinate.}
\]

Next, we make the common approximation that well-developed, steady flow proceeds at constant volume, so that \( \dot{\gamma}_{kk} = 0 \) [10, 32, 41, 66] and define the equivalent shear strain-rate as \( \dot{\gamma} = (2\dot{\gamma}_{ij}\dot{\gamma}_{ij})^{1/2} \). The Cauchy stress tensor and stress deviator are denoted as \( \sigma_{ij} = \sigma_{ji} \) and \( \sigma'_{ij} = \sigma_{ij} - (1/3)(\sigma_{kk})\delta_{ij} \). Then, the equivalent shear stress, pressure, and stress ratio are defined through stress-tensor invariants as \( \tau = (\sigma'_{ij}\sigma'_{ij}/2)^{1/2}, \quad P = -\sigma_{kk}/3, \) and \( \mu = \tau / P \), respectively. Finally, assuming that the strain-rate tensor and stress deviator are codirectional [10, 32, 66], the one-dimensional flow rule (2.3) may be expressed in tensorial form as

\[
\sigma_{ij} = -P\delta_{ij} + 2\frac{P}{g}\dot{\gamma}_{ij}. \tag{2.4}
\]

We note that codirectionality is an approximation, and slight deviations from codirectionality have been observed in discrete element simulations – namely \( \sim 1-2\% \) non-coaxiality between \( \dot{\gamma}_{ij} \) and \( \sigma'_{ij} \) [68] and the normal stress differences [69]. However, codirectionality remains a useful simplifying assumption and enables a reasonably good description of experimental data. For recent work incorporating these effects into a rheological model, see Weinhart et al. [68].

\*Recent work has shown that dilatancy can have an effect on steady flows, leading to secondary flow with magnitude on the order of \( \sim 5\% \) of the primary flow [67]. Since this effect has not yet been reported for steady, dense granular heap flow, we neglect it in the present work.
3. **Nonlocal rheology**: With the introduction of the granular fluidity field, $g$, an additional field equation is required to relate the fluidity field to the stress field. In a local constitutive approach, the fluidity would be given as an algebraic function of the stress through the stress invariants $\mu$ and $P$. In contrast, in the nonlocal approach, the granular fluidity, $g$, is governed by the following partial differential equation\(^6\):

$$
\frac{Dg}{Dt} = A^2 d^2 \frac{\partial^2 g}{\partial x_k \partial x_k} - \left[ \Delta\mu \left( \frac{\mu_s - \mu}{\mu_2 - \mu} \right) g + b \sqrt{\rho_s d^2 P \mu g^2} \right],
$$

(2.5)

where $D(\bullet)/Dt$ is the material time derivative\(^5\). In (2.5), $t_0$ is a constant timescale associated with the dynamics of $g$, $A$ is a constant dimensionless material parameter characterizing nonlocal effects called the nonlocal amplitude, and the constants $\Delta\mu = \mu_2 - \mu_s$ and $b = \Delta\mu / I_0$ are given through the three constant material parameters \{$\mu_s, \mu_2, I_0$\} appearing in the local inertial rheology (2.1). The mean grain diameter and grain material density continue to be denoted by $d$ and $\rho_s$, respectively, and are constants. During steady, homogeneous flow, the nonlocal rheology (2.5) reduces to the local inertial rheology, (2.1) and (2.2). To see this, consider homogenous flow in the absence of spatial gradients in $g$ ($\partial^2 g / \partial x_k \partial x_k = 0$) and for a fixed state of stress $(\mu, P)$. Then, at sufficiently long time ($t \gg t_0$), $g$ evolves to a stable Lagrangian steady state ($Dg/Dt \approx 0$), which we denote as $g_{\text{loc}}(\mu, P)$. The nature of the stable steady state, $g_{\text{loc}}(\mu, P)$, depends on the sign of $(\mu_s - \mu)$. For $\mu \leq \mu_s$, the only steady solution is $g_{\text{loc}} = 0$, and it is stable under perturbation in $g$. For $\mu > \mu_s$, $g_{\text{loc}} = 0$ remains a steady solution; however, it becomes unstable under perturbation in $g$. The stable, steady solution for $\mu > \mu_s$ is $g_{\text{loc}} = \sqrt{P / \rho_s d^2 I_0 (\mu - \mu_s) / (\mu (\mu_2 - \mu))}$.\(^5\)

\(^5\)Note that the nonlocal rheology (2.5) shows mathematical similarities to the order-parameter-based rheological approach of Aranson and Tsimring\(^{46}\).
Putting the stable solutions together, we have

\[
g_{\text{loc}}(\mu, P) = \begin{cases} 
\sqrt{P/\rho_s d^2} I_0 \frac{(\mu - \mu_s)}{\mu (\mu_2 - \mu)} & \text{if } \mu > \mu_s, \\
0 & \text{if } \mu \leq \mu_s.
\end{cases}
\]  

(2.6)

We call the stress-dependent function \(g_{\text{loc}}(\mu, P)\) the local fluidity, since if the granular fluidity, \(g\), is taken to be given through the function \(g_{\text{loc}}(\mu, P)\) and combined with the flow rule (2.4), we recover the local inertial rheology, (2.1) and (2.2). Then, in the case of inhomogeneous flows involving spatial gradients in \(g\), the Laplacian term appearing in (2.5) introduces an intrinsic length scale given through \(d\), and hence, the rheology is nonlocal in character. In the present work, we are concerned with dense granular flows that are steady in a Lagrangian sense, in which \(t \gg t_0\) so that \(Dg/Dt \approx 0\). However, reducing the dynamical PDE (2.5) to the steady-state case is not as simple as setting the left-hand side to zero because the stability of the \(g = 0\) solution depends on the sign of \((\mu_s - \mu)\). In order to obtain a differential relation for \(g\) specialized to the case of steady flow, we allow for gradients in \(g\) but limit attention to small deviation of \(g\) from \(g_{\text{loc}}\) for a given state of stress \((\mu, P)\). The result of such a simplification (see Section 4.3.1 of Henann and Kamrin [60] for the details of this calculation) is

\[
g = g_{\text{loc}} + \xi^2 \frac{\partial^2 g}{\partial x_k \partial x_k},
\]  

(2.7)

where \(g_{\text{loc}}(\mu, P)\) is the local fluidity function, given through \((\mu, P)\) as in (2.6), and \(\xi(\mu)\) is a stress-dependent length-scale called the cooperativity length, given by

\[
\xi(\mu) = A \sqrt{\frac{\mu_2 - \mu}{\Delta \mu |\mu - \mu_s|} d}.
\]  

(2.8)
Note that in the absence of any stress or flow gradients \( \partial^2 g/\partial x_k \partial x_k = 0 \), the steady-state form (2.7) simply reduces to \( g = g_{\text{loc}}(\mu, P) \), and the local inertial rheology is recovered, as should be the case for homogeneous, steady flow. However, for inhomogeneous flow, the presence of the Laplacian term gives rise to nonlocal effects – with predictions of the NGF model being size-dependent due to the cooperativity length (2.8) being directly proportional to the grain size, \( d \). In particular, in regions where \( \mu \leq \mu_s \), the local fluidity (2.6) is zero, and (2.7) reduces to \( g = \xi^2 (\partial^2 g/\partial x_k \partial x_k) \), which gives rise to creeping flow predictions with a decay length determined by \( \xi \) rather than a sharp flow cutoff. In the simulations of Section 2.3, with a few noted exceptions, we utilize the steady-state form of the NGF model, (2.7) with (2.6) and (2.8), rather than the dynamical form (2.5). We note that the dimensionless parameter \( A \) appearing in (2.8) is the only new material parameter introduced in the steady-state form of the NGF model beyond the local parameters, \( \{ \mu_s, \mu_2, I_0 \} \).

The system of equations described above are then closed by the standard equations of motion

\[
\frac{\partial \sigma_{ij}}{\partial x_j} + \phi \rho_s G_i = \phi \rho_s \frac{Dv_i}{Dt} \tag{2.9}
\]

with \( G_i \) the acceleration of gravity (denoted as \( G \) to differentiate it from the granular fluidity \( g \)) and \( \phi \) the solid volume fraction, taken to be 0.62 for randomly-closed-packed, quasi-monodisperse, spherical grains [70]. Consistent with our assumption of steady, well-developed flow, we neglect the effect of macroscopic inertia, so that (2.9) reduces to

\[
\frac{\partial \sigma_{ij}}{\partial x_j} + \phi \rho_s G_i = 0_i. \tag{2.10}
\]

The boundary conditions accompanying this boundary-value problem are discussed in the next section in the context of the specific problem of steady, dense granular heap flow.

In previous work, the NGF model has been shown to quantitatively describe a broad set of experimental steady flow data, including all variations of the complex split-bottom
family of geometries in addition to annular shear flow and planar shear flow with gravity [28]. The model has also been shown to correctly capture other nonlocal phenomena such as nonlocally-induced material weakening, i.e., “secondary rheology” [17, 29], whereby the motion of a boundary removes the yield strength of the material everywhere, permitting far-away loaded objects to creep through the grains when otherwise they would remain static [57]. Finally, in Kamrin and Henann [58], the model has also shown itself able to describe the size-dependent strengthening seen in experiments of gravity-driven flow down a rough inclined plane [11, 30, 31] – a problem that we will consider further in Chapter 3. When discussing the successes of the NGF model, it is also important to note its limits. Although the NGF model can model developing flows and the approach to steady state, it has not been designed to be quantitatively predictive in this regard. In particular, it is not yet known whether the time-dependent term appearing in the dynamical form (2.5) is able to quantitatively capture transient effects, such as those reported by Ries et al. [71]. Hence, at present, the NGF model is only appropriate for steady-state conditions. It is also limited to granular systems, in which grains are spherical, quasi-monodisperse, and stiff. In what follows, we will apply the model to situations in which these assumptions are valid.

2.3 Numerical simulations of dense, steady granular heap flow

In this section, we turn to applying the NGF model to the problem of dense, steady granular heap flow. We will compare predictions of the NGF model to experiments in the literature using glass beads [24, 25]. Regarding the dimensionless material parameters for glass beads \{\mu_s, \mu_2, I_0, A\}, the local parameters are taken from well-established data [9, 59]:

\[
\mu_s = 0.3819, \quad \mu_2 = 0.6435, \quad \text{and} \quad I_0 = 0.279.
\]
In previous work \[28\], the nonlocal amplitude for glass beads was calibrated to be

\[ A = 0.48 \]

by fitting NGF model predictions to experimental flow fields for dense, quasi-static granular flow in the split-bottom cell \[13, 14\]. Since the heap flows reported by Jop and coworkers \[24, 25\] also involve dense flows of spherical glass beads, we expect that these material parameter values remain valid, and \textit{in what follows, we continue to use these parameters without adjustment}. Further, we take \( \rho_s = 2450 \text{ kg/m}^3 \) and \( d = 0.5 \text{ mm} \) in our calculations; however, all results in subsequent sections will be presented in dimensionless form, and hence, the numerical values of \( \rho_s \) and \( d \) are inconsequential.

### 2.3.1 Flow configuration

To study gravity-driven, dense granular heap flow, we consider the system shown in Fig. 2.1(a), consisting of a granular layer of depth, \( H \), at an inclination angle, \( \theta \), flowing between two smooth, frictional side walls separated by a distance, \( W \). The coefficient of sliding friction between the granular media and the side walls, \( \mu_{\text{wall}} \), is taken to be a constant value and the floor is rough. The component of the acceleration of gravity in the \( y \)-direction \( -G \sin \theta \) – then drives flow down the channel – which is very long in the \( y \)-direction. The expected consequent steady-state flow field – which is invariant along the length of the channel, i.e., the \( y \)-direction, and decays with depth beneath the surface, i.e., the \( z \)-direction – is sketched schematically in Fig. 2.1(a). The total volume flow-rate of granular material down the channel is denoted by \( Q \). Note that in experiments the flow-rate, \( Q \), is typically prescribed, and the free surface inclination angle, \( \theta \), follows as a consequence \[9\].

To apply the NGF model to flow in this configuration, we take advantage of the invariance of the steady flow field in the \( y \)-direction and make an antiplane shear idealization,\[6\]

\[6\] In the present work, we use \( Q \) to denote the total volume flow-rate, rather than the flow-rate per unit width as in Jop et al. \[9, 25\].
in which the only non-zero component of velocity is in the y-direction, denoted by $v$, and only depends on the $x$ and $z$ coordinates, i.e., $v(x, z)$, thereby reducing the problem to two dimensions. Under the antiplane shear assumption, the constitutive equation (2.4) implies that the non-zero stress components are $\sigma_{xx} = \sigma_{yy} = \sigma_{zz} = -P$, $\sigma_{xy} = (P/g)\partial v/\partial x$, and $\sigma_{yz} = (P/g)\partial v/\partial z$, and hence for steady ($Dv_i/Dt = 0$) antiplane shear flow, the pressure field is simply hydrostatic, $P(z) = \phi\rho_s G(\cos \theta)z$, and the one remaining equilibrium equation (2.10) reduces to

$$\frac{\partial \sigma_{xy}}{\partial x} + \frac{\partial \sigma_{yz}}{\partial z} + \phi\rho_s G(\sin \theta) = 0. \quad (2.11)$$

The fields $v(x, z)$ and $g(x, z)$ may be solved through the coupled partial differential equations (2.7) and (2.11) along with appropriate boundary conditions. Solutions to this boundary-value problem are obtained via the custom finite-element approach, described in Henann and Kamrin [72] and implemented in the commercial finite-element program Abaqus [73]. In the implementation, a stiff elastic response is included, which does not affect the calculated steady flow fields, and as such, the finite-element degrees-of-freedom are the displacement in the $y$-direction – rather than $v$ – and the granular fluidity. For details on this point, see Henann and Kamrin [72]. A sample computational domain for the case of $W = 19d$ and $H = 20d$ is shown in Fig. 2.1(b). Based on the mesh convergence study for
the finite-element implementation described in Henann and Kamrin [72], we choose a fine mesh resolution of $0.125d$ to ensure accurate calculation results.

Regarding mechanical boundary conditions – indicated in Fig. 2.1(b) – the top surface is traction-free, $\sigma_{yz}(x) = 0$ at $z = 0$, the side walls are frictional, $\sigma_{xy}(z) \leq -\mu_{\text{wall}} \sigma_{xx}(z) = \mu_{\text{wall}} P(z)$ at $x = 0$ and $x = W$, and the bottom is rough, $\nu(x) = 0$ at $z = H$. Regarding the frictional side wall boundary condition, as in the bulk, there is a stiff elastic component to the wall slip, so that the shear traction on the granular media at a point on the surface, $\sigma_{xy}(z)$, may be less than $\mu_{\text{wall}} P(z)$; however, for steady wall slip, $\sigma_{xy}(z) = \mu_{\text{wall}} P(z)$. Throughout, we take a constant value of the wall friction coefficient of $\mu_{\text{wall}} = 0.32$, obtained by treating $\mu_{\text{wall}}$ as an adjustable parameter in our subsequent comparisons with experiments. More specifically, as will be pointed out in Section 2.3.3, $\mu_{\text{wall}}$ is determined by fitting to the overall flow-rate data of Fig 2.4(a) rather than any specific flow field. Note that since the material parameters $\{\mu_s, \mu_2, I_0, A\}$ have been previously calibrated to experimental flow fields in other flow configurations and subsequently fixed, $\mu_{\text{wall}}$ represents the only adjustable parameter in our simulations of dense heap flow. This simple picture of side wall friction is an idealization [see 74, 75]. In particular, the recent work of Artoni and Richard [75] has shown that the sliding friction coefficient is not constant. Instead, it depends on both the slip velocity as well as the velocity fluctuation, $\delta \nu$. In spite of this simplification, our comparisons with experiments will show that good agreement may still be obtained under this idealization. For the granular fluidity boundary conditions, we invoke homogeneous Neumann boundary conditions on all boundaries. This is based on past work, which has shown that such a boundary condition provides an excellent description of experiments, provided that the size of the flow geometry is greater than approximately $10d$ (see Henann and Kamrin [72] for an expanded discussion of this point).
Figure 2.2: Flow fields in a narrow channel of width $W/d = 19$. Contour plots of the normalized, steady-state velocity field, $v/\sqrt{Gd}$, in the $x$-$z$-plane for (a) $\theta = 26.1^\circ$ and (b) $\theta = 28.0^\circ$ calculated using the steady-state NGF model \((2.7)\). Normalized velocity field at the wall, $v_{\text{wall}}/\sqrt{Gd}$, as a function of the depth beneath the free surface, $z$, for each surface inclination angle, $\theta$, in (c) linear and (d) semi-logarithmic scale. Symbols represent the experimental data of Jop et al.\cite{25}; solid lines are the calculated results of the steady-state NGF model \((2.7)\); dotted lines are the calculated steady results of the dynamical NGF model \((2.5)\); and dashed lines are the calculated results of the local inertial rheology \((2.2)\).

### 2.3.2 Flow fields

In this section, we compare simulated flow fields with experiments. To do so, we must first specify the geometry – most importantly, the dimensionless channel width, $W/d$. Throughout, we take the depth of the granular layer, $H/d$, to be large enough that it does not affect the flow field. Second, we must specify either the inclination of the free surface, $\theta$, or the volume flow-rate, non-dimensionalized as $Q/Wd\sqrt{Gd}$\footnote{This dimensionless flow-rate is denoted as $Q^*$ in Jop et al.\cite{9,10}.}

Following the experiments of Jop et al.\cite{25}, we begin by considering narrow channels of width $W/d = 19$ for two values of the free surface inclination angle – $\theta = 26.1^\circ$ and $\theta = 28.0^\circ$ – and calculate steady flow predictions using the steady-state form of the NGF model \((2.7)\) and the computational setup of Fig. 2.1(b). Contour plots of the normalized velocity...
field at steady state, $v/\sqrt{Gd}$, in the x-z-plane for each case are shown in Figs. 2.2(a) and (b). As expected, flow is at its most rapid at the free surface with the velocity decaying into the bulk (in the z-direction). In the cross-channel direction (the x-direction), the velocity field has a clear bowed shape due to the frictional side walls. As is clear from the contour plots of Figs. 2.2(a) and (b), flow for the $\theta = 28.0^\circ$ case is considerably more rapid. For the purpose of comparing to experiments, we introduce the wall velocity field, $v_{\text{wall}}(z)$, at an x-position of $x = d –$ one grain diameter inside the side wall. Figure 2.2(c) displays the good quantitative agreement between the simulated wall flow fields (solid lines) and the experimental data of Jop et al. [25] (symbols) for the two inclination angles considered. In particular, the NGF model captures both the rapid flow near the free surface as well as the exponentially-decaying, creeping velocity field deep beneath the surface – made clear in the semi-logarithmic-scale plot of the wall velocity field in Fig. 2.2(d).

For comparison, we have also calculated steady flow predictions of the dynamical form of the NGF model (2.5) in a narrow channel of width $W/d = 19$. To obtain steady flow predictions for the dynamical form of the NGF model, an initial condition for the fluidity field, $g$, is required due to the presence of the time derivative in (2.5). Since steady ($t \gg t_0$) solutions of the dynamical form of the NGF model (2.5) are expected to be similar to the solutions of the steady-state NGF model (2.7), we utilize the respective solutions of the steady-state form as the initial condition for the dynamical form for each case. Then, we choose an arbitrary value of the timescale $t_0$ and run the simulation to a final time of $1000t_0$ to ensure that the steady state is attained. The material parameters and boundary conditions remain unchanged. The calculated steady wall velocity fields for the dynamical form of the NGF model for the cases of $\theta = 26.1^\circ$ and $\theta = 28.0^\circ$ are included in Figs. 2.2(c) and (d) as dotted lines. For both free surface inclination angles, the calculated steady predictions of both forms of the NGF model are quite similar in both the rapidly-flowing surface layer and the creeping bulk. Since solutions are much more easily obtained through the steady-state form of the NGF model (2.7), it is typically preferable to use this form in practice.
As a second comparison, we have calculated steady flow predictions of the local inertial rheology (2.2) in a narrow channel of width \( W/d = 19 \). Steady flow predictions of the local inertial rheology (2.2) are obtained by setting the nonlocal amplitude to zero, i.e., \( A = 0 \), and leaving all other material parameters and boundary conditions unchanged. The calculated wall velocity fields for the local inertial rheology for the cases of \( \theta = 26.1^\circ \) and \( \theta = 28.0^\circ \) are plotted in Figs. 2.2(c) and (d) as dashed lines. In the rapidly flowing surface layer, the NGF model and the local inertial rheology offer similar flow field predictions, which are both in agreement with experimental data. However, beneath the surface, the local inertial rheology predicts a sharp flow cutoff, clearly observed in the semi-logarithmic-scale plot of Fig. 2.2(d), whereas the NGF model is capable of capturing the exponentially-decaying, creeping bulk. The NGF model clearly provides significantly improved predictions of steady, dense granular heap flow fields compared to the local inertial rheology.

Next, returning to the steady-state NGF model (2.7), we consider a wider channel with \( W/d = 142 \) and compare to the experimental data of Jop [24]. For this set of experiments, the flow-rate, \( Q/W d \sqrt{Gd} \), was reported rather than the inclination angle, \( \theta \). Accordingly, we consider flow-rates of \( Q/W d \sqrt{Gd} = 4.4, 15, 40, \) and 91.8 Contour plots of the normalized, steady-state velocity field, \( v/\sqrt{Gd} \), in the \( x-z \)-plane are shown in Fig. 2.3(a) and (b) for the least rapid and most rapid flow-rates, \( Q/W d \sqrt{Gd} = 4.4 \) and 91, respectively. Again, we observe that the velocity decays with the depth beneath the surface and is greater in the center of the channel than at the walls. In the contour plots, it is clear that the size of the rapidly-flowing surface layer is larger for the higher flow-rate. Figure 2.3(c) then shows the comparison of the calculated wall velocity field, \( v_{\text{wall}}(z) \), to the experimental data of Jop [24] for all four volume flow-rates, and again the quantitative agreement is good both for the rapid flow near the surface as well as the creeping bulk. Defining the surface flow

---

8In our calculations, the inclination angle, \( \theta \), is prescribed, so for the \( W/d = 142 \) simulations, \( \theta \) is iteratively adjusted to achieve the desired volume flow-rate. We utilize a channel depth of \( H/d = 140 \) and a mesh resolution of 0.5\( d \).
Figure 2.3: Flow fields in a wide channel of width \( W/d = 142 \). Contour plots of the normalized, steady-state velocity field, \( v/\sqrt{Gd} \), in the \( x-z \)-plane for (a) \( Q/Wd\sqrt{Gd} = 4.4 \) and (b) \( Q/Wd\sqrt{Gd} = 91 \) calculated using the NGF model. (c) Normalized velocity field at the wall, \( v_{\text{wall}}/\sqrt{Gd} \), as a function of the depth beneath the free surface, \( z \), and (d) normalized velocity field on the surface, \( v_{\text{surf}}/\sqrt{Gd} \), as a function of \( x \) for each volume flow-rate, \( Q/Wd\sqrt{Gd} \). Symbols represent the experimental data of Jop [24], and solid lines are the calculated results of the steady-state NGF model.

Field as \( v_{\text{surf}}(x,z=0) \), Fig. 2.3(d) shows that the calculated surface flow field is also in agreement with experiments – both at the wall and in the center of the channel. Overall, the NGF model is able to capture the salient aspects of the flow fields in steady, dense granular heap flow over a range of channel widths.

### 2.3.3 Volume flow-rate and maximum velocity

Additional insight may be obtained by comparing the predicted relationships between global quantities – such as the relationships between volume flow-rate, \( Q \), maximum velocity, \( v_{\text{max}} = v(x=W/2,z=0) \), and free surface inclination angle, \( \theta \) – to experiments. Before making such comparisons, we first consider some consequences of dimensional analysis. The dense granular heap flow configuration of Fig. 2.1(a) relates the following quantities – \( W, \ d, \ \rho_s, \ \rho_sG, \ \text{and} \ \theta \) – to the consequent volume flow-rate, \( Q \), and maximum velocity,
Figure 2.4: Relationships between (a) free surface inclination angle, $\theta$, and dimensionless volume flow-rate, $Q'$, and (b) dimensionless maximum velocity, $v_{\text{max}}'$, and dimensionless flow-rate, $Q'$, for steady, dense granular heap flow. Symbols represent the experimental data of [9], and lines are calculated predictions of the steady-state NGF model.

$v_{\text{max}}$. However, the analysis of Jop et al. [9] showed that the scaling suggested by the local inertial rheology (2.1) could account for the observed scalings between $Q$, $v_{\text{max}}$, and $\theta$, and importantly, in the local inertial rheology, the grain size does not appear independently – instead combined with the grain material density as $\rho_s d^2$. Consequently, the reduced set of quantities – $W$, $\rho_s d^2$, $\rho_s G$, and $\theta$ – should give $Q$ and $v_{\text{max}}$. Straightforward dimensional analysis leads to the conclusion that the local inertial rheology suggests a one-to-one relationship between the following three dimensionless quantities:

$$Q' = \frac{Q d}{G^{1/2} W^{7/2}}, \quad v_{\text{max}}' = \frac{v_{\text{max}} d}{G^{1/2} W^{3/2}}, \quad \text{and} \quad \theta.$$

Such a collapse was observed in experimental data by Jop et al. [9], and their data in the form $\tan \theta$ versus $Q'$ and $v_{\text{max}}'$ versus $Q'$ is reproduced in Figs. 2.4(a) and (b), respectively, for several channel widths. Also plotted in Fig. 2.4 are the respective calculated relationships obtained from the NGF model for $W/d = 19$ and 142 – both a narrow and a wide channel. We note that the constant wall friction coefficient, $\mu_{\text{wall}}$, was determined by fitting to the data of Fig. 2.4(a), rather than by fitting to individual flow fields of Section 2.3.2. We observe first that agreement with experiments may be obtained as a result. Second, while the local inertial rheology predicts a perfect collapse between $Q'$, $v_{\text{max}}'$, and $\theta$, the collapse for the NGF model is approximate with the differences between the simulated relationships
for the two channel widths being small, indicating that nonlocal effects – i.e., the presence of the creeping bulk – are secondary in these scaling relationships. Therefore, the NGF model is able to account for the most significant deficiency in the predictions of the local inertial rheology applied to steady, dense heap flow – i.e., the existence of the creeping bulk – while approximately maintaining its greatest success – i.e., the scalings between $Q'$, $v'_\text{max}$, and $\theta$.

### 2.3.4 Two length scales

Finally, to explore the qualitative difference between the rapidly-flowing surface layer and the creeping bulk, we introduce two characteristic length scales. Following Jop et al. [25], the rapidly-flowing surface layer is characterized by the mean flow depth, $h$, defined as $h = Q/W v'_\text{max}$. The creeping bulk is characterized by the decay length of the exponential tail in the mid-channel velocity field, $\lambda$, defined through $v(x = W/2, z) \sim \exp(-z/\lambda)$ for large $z$. Figure 2.5(a) shows both $h/d$ and $\lambda/d$ versus the dimensionless flow-rate, $Q'$, for the calculated results of the NGF model for $W/d = 19$. Importantly, $h$ is flow-rate-dependent while $\lambda$ is flow-rate-independent, which agrees both qualitatively and quantitatively with experiments (see Fig. 4(b) of Jop et al. [25] in which $\lambda/d$ extracted from the wall flow field is approximately 2 for $W/d = 19$). This observation may be understood mathematically
as follows. In the rapidly-flowing layer where \( \mu > \mu_s \), the local contribution to (2.7), \( g_{\text{loc}} \), dominates, introducing the rate-dependence of the local rheology. Conversely, in the creeping bulk where \( \mu < \mu_s \), \( g_{\text{loc}} = 0 \), rendering (2.7) rate-independent [27] and leading to the rate-independence of \( \lambda \). Regarding the dependence of the length scales \( h \) and \( \lambda \) on the channel width \( W \), since \( h \) is defined through \( Q \) and \( v_{\text{max}} \), its scaling may be understood through the arguments of Section [2.3.3]; however, due to the rate-independence of \( \lambda \), we expect that \( \lambda / d \) will only depend upon \( W / d \) (see Figure 2(b) of Henann and Kamrin [28] for the analogous relationship between a flow length scale and geometry in split-bottom flow). Figure [2.5(b) shows \( \lambda / d \) versus \( W / d \) calculated by the NGF model for channel widths ranging from \( W / d = 12 \) to 142. The observed relationship appears close to a 1/4 power-law (plotted as a dashed line for reference); however, appropriate experimental data to verify this point has not been reported.

### 2.4 Concluding remarks

In this chapter, we have shown that the NGF model is capable of capturing several important experimentally-observed aspects of steady, dense granular heap flow, including (i) wall and surface flow fields for a range of channel widths; (ii) the relationships between volume flow-rate, maximum velocity, and surface inclination; and (iii) the rate-dependent thickness of the rapidly-flowing surface layer and the rate-independent decay length of the exponentially-decaying velocity field in the creeping bed. Importantly, the NGF model offers improved flow predictions over the local inertial rheology while involving only one new dimensionless material parameter, the nonlocal amplitude \( A \). In previous work, the value of \( A \) for glass beads was determined by applying the NGF model to slow boundary-driven flows [28], and in the present work, we have continued to use this numerical value and demonstrated that good agreement with experiments is maintained in the case of steady, dense granular heap flow.
There remain several avenues for improvement and refinement. A major idealization of our modeling work is treating the friction coefficient between the granular material and the side walls as constant – instead of dependent on the slip velocity and velocity fluctuation as shown by Artoni and Richard [75]. The recent work of [64] relating the granular fluidity to the velocity fluctuation suggests a path forward on this point, in which the wall friction coefficient is taken to be dependent on both the slip velocity and the granular fluidity.

We have limited attention to the case of steady, well-developed flow. To apply the NGF model to transient, developing flows, the incorporation of additional physics is required. The work of Jop et al. [25] showed that accounting for macroscopic inertia in conjunction with the local inertial rheology was sufficient to obtain a reasonable description of the approach to steady state in dense granular heap flow, quantified by the overall flow rate and free surface velocity as a function of time. Since the inertial rheology and the NGF model provide comparable predictions in the rapid flow regime, if macroscopic inertia effects are reintroduced to (2.11), we expect to obtain similar results with the NGF model. Transient effects are not solely due to macroscopic inertia. For example, Reynolds dilation during shear initiation induces transient variations in the flow resistance, which are commonly described using critical-state models [76] but which are not yet included in the NGF model. Further, Ries et al. [71] recently reported an exponential-type transient during the initiation of dense simple shearing of spheres, and it is not yet known whether this transient may be captured using the time-dependent, dynamical form of the nonlocal rheology (2.5).

In closing, the ability of the NGF model to capture steady, dense granular heap flow in a channel is an encouraging indication that the model might successfully be applied to other types of surface flow, such as the flows that arise in rotating drums. The essential physics of steady, dense granular flow in a rotating drum is expected to be the same as that in channel flows [7], but the geometric complexity of the rotating drum configuration gives rise to additional characteristics in the flow field, such as the S-shape of the free surface. Applying the NGF model to steady, dense flows in a rotating drum will possibly require
more elaborate numerical techniques than the finite-element-based approach, such as the material point method [35] [37], and is a task which is left to future work.
Chapter 3

Size-dependence of the flow threshold in dense granular materials

Note: A version of this chapter is published in Soft Matter. Data and figures have been used with all co-authors’ consent.


3.1 Introduction

Recall from the discussion of Section 2.1 that the local inertial rheology relates the inertial number \( I \) and the stress ratio \( \mu \) through a one-to-one functional relationship \( \mu = \mu_{loc}(I) \), which is empirically fit. A common feature among different functional forms of the inertial rheology is a static yield value of the stress ratio – \( \mu_{loc}(I \to 0) = \mu_s \). Consequently, the inertial rheology possesses a flow threshold in which steady flow is not possible when \( \mu < \mu_s \) but steady flow becomes possible whenever \( \mu \) exceeds \( \mu_s \).

\[ ^1 \text{In the common generalization of the inertial rheology to three-dimensions} \ [10, 32], \text{the flow threshold takes the form of a Drucker-Prager yield condition} \ [38]. \]
A logical next step is to apply this flow threshold to more complex flow configurations. A dense granular flow configuration that is more complex than homogeneous, planar shear – but still quite simple – is flow down a rough inclined surface, shown schematically in Fig. 3.1(a). In inclined plane flow, the ratio of the shear stress to the pressure is a constant value at every point in the granular layer – as in planar shear – and is given through the inclination angle $\theta$ by $\mu = \tan \theta$. Therefore, the flow threshold associated with the inertial rheology predicts that flowing and non-flowing states are separated by a thickness-independent angle of repose $\theta_r = \tan^{-1} \mu_s$. However, extensive experiments and discrete-element method (DEM) simulations have shown that this is not the case [7, 11, 30, 31, 59, 77]. Instead, thin granular layers do not flow for a range of $\theta$ greater than $\theta_r$ with additional strengthening as the layer thickness is decreased. This observation is illustrated in Fig. 3.1(b) for experimental measurements of glass beads on a fully rough base, reported by Pouliquen [11].

The inability of the inertial rheology to capture this size effect stems from its local nature – local in the sense that it relates the stress state to the strain-rate at a point. The size-dependence of the flow threshold in inclined plane flow arises due to nonlocal, cooperative effects at the microscopic grain level, which are not accounted for in the inertial
rheology. In a thin granular layer, the proximity of the grains to the fixed, rough, inclined surface imbues the granular layer with additional strength. The converse manifestation of cooperativity may also be observed. Flow in one region of a granular medium can induce flow in far-away regions – even when these regions experience stress states that are beneath the flow threshold extracted from homogeneous, planar shearing. For example, as discussed in Chapter 2 in gravity-driven heap flow, a decaying flow field is observed, whereas the stress-based flow threshold of the inertial rheology would predict a sharp flow cutoff. An additional example of this effect is the “secondary rheology” of intruders, whereby the motion of a boundary removes the flow threshold of the material everywhere, permitting far-away loaded objects to creep through the grains when otherwise they would remain static [29].

While the effect of cooperativity on steady flow fields has been investigated in a diverse set of geometric configurations, studies exploring the size-dependence of the flow threshold in dense granular materials have been limited to inclined plane flow. To better elucidate the role of the stress field, the first purpose of this chapter is to systematically explore the size-dependence of the flow threshold in different flow configurations with more complex stress fields. Specifically, we consider dense two-dimensional flows of stiff, frictional disks using DEM simulations in three flow configurations: (1) planar shear flow with gravity, (2) annular shear flow, and (3) vertical chute flow, and show that additional strengthening is observed as the system size is reduced in all three cases.

The second purpose of this chapter is to rationalize the dependence of the flow threshold on the system size in the presence of different stress fields with the nonlocal granular fluidity (NGF) model. Among the various nonlocal continuum constitutive theories proposed in the literature, several have been applied to the flow threshold in inclined plane flow, such as integral equations representing a self-activated process [45]; Ginzberg-Landau theories based on a partial-fluidization order parameter [46] or the inertial number [54]; and extensions of kinetic theory [48]. The NGF model has also been shown to be capable of
capturing the size-dependence of the flow threshold in inclined plane flows of glass beads \[58\] – as illustrated in Fig. 3.1(b). In this chapter, we utilize the NGF model to obtain predictions of the size-dependence of the flow threshold in planar shear flow with gravity, annular shear flow, and vertical chute flow. Specifically, in each case, we calculate the analytical flow threshold predicted by the NGF model. Importantly, we show that the NGF model is capable of quantitatively describing the observed size-dependent strengthening in all three flow configurations, while simultaneously capturing steady flow fields.

The remainder of this chapter is organized as follows. In Section 3.2, we discuss the specifics of our two-dimensional DEM simulations and verify our simulations against existing DEM data for stiff, frictional disks in planar shear flow from the literature \[8,78\]. In Section 3.3, we discuss the NGF model and its attendant description of the flow threshold. Then, in Section 3.4, we present the results of our DEM simulations in planar shear flow with gravity, annular shear flow, and vertical chute flow along with the predictions of the NGF model, comparing predictions of both the size-dependent flow threshold and steady flow fields to DEM data. We close with discussion and concluding remarks in Section 3.5.

### 3.2 Discrete-element method simulations

In this section, we provide details of our two-dimensional DEM methodology and briefly describe simulations of planar shear flow in order to verify our simulations against existing literature data \[8,78\].

#### 3.2.1 Simulated granular system

Following several previous works \[8,27,41,78\], we consider a simulated, two-dimensional, quasi-mondisperse granular system consisting of a dense collection of dry, stiff, frictional, circular disks.\(^2\) The average disk diameter and the grain-material area-density are denoted

\(^2\)This is in contrast to the discussion of Chapter 2 which focused on dense collections of spheres.
as \( d \) and \( \rho_s \), respectively, so that we may define a characteristic grain mass as 
\[
m = \rho_s \pi d^2 / 4.
\]
In our DEM simulations, the distribution of disk diameters involves a polydispersity of 
\( \pm 20\% \) to prevent crystallization. In the context of disks, the inertial rheology then relates 
the stress state – specifically, the pressure \( P \) and the shear stress \( \tau \) (both with units of force 
per length in two-dimensional settings) – to the consequent shear strain-rate \( \dot{\gamma} \). Nondimensional-
izationalizing the aforementioned quantities gives the inertial number 
\[
I = \dot{\gamma} \sqrt{m / P}
\]
and the stress ratio \( \mu = \tau / P \). While the form of the inertial number is slightly modified for two-
dimensional disks when compared to the form used for three-dimensional spheres, it still 
represents the ratio of the microscopic time-scale associated with particle motion \( \sqrt{m / P} \) 
to the macroscopic time-scale of applied deformation \( 1 / \dot{\gamma} \).

We utilize a standard DEM grain interaction model \[8\]. Specifically, there is no force 
between non-overlapping grains, but when two grains overlap, they interact through a 
spring/dashpot contact law that accounts for elasticity, damping, and sliding friction. With 
\( \delta_n \geq 0 \) and \( \delta_t \) denoting the normal and tangential components of the contact displace-
ment, the normal contact force \( F_n \) is given linearly through the normal contact displace-
ment with stiffness \( k_n \) and the relative normal velocity with damping coefficient \( g_n \), i.e., 
\[
F_n = k_n \delta_n + g_n \dot{\delta}_n.
\]
The normal damping coefficient is specified through the coefficient of 
restitution for binary collisions \( e \) by 
\[
g_n = \sqrt{mk_n(-2 \ln e)} / \sqrt{2(\pi^2 + \ln^2 e)}.
\]
Tangential inter-
actions are described by a stiffness \( k_t \) and damping coefficient \( g_t \), which we take to be zero, 
so that the tangential contact force is \( F_t = k_t \delta_t \). Importantly, the tangential contact force is 
limited by Coulomb friction, described by the inter-particle sliding friction coefficient \( \mu_{surf} \). 
Therefore, grain interactions are fully described through the parameter set \( \{k_n, k_t, e, \mu_{surf}\} \). 
In order to simulate stiff, quasi-rigid grains, the normal stiffness is taken to be sufficiently 
large throughout, i.e., \( k_n / P > 10^4 \), where \( P \) is the characteristic confining pressure for a 
given flow configuration. Next, it is well-appreciated that the precise values of \( k_t / k_n \) and \( e \) 
have a negligible impact on the phenomenology of dense flows of stiff disks \[8\], and as in
Figure 3.2: (a) Configuration for two-dimensional DEM simulations of planar shear flow. Black grains denote rough walls, and gray grains denote flowing grains. (b) The local inertial rheology – $\mu$ versus $I$ – for frictional disks with inter-particle sliding friction coefficient of $\mu_{\text{surf}} = 0.4$. Black symbols denote the DEM data of da Cruz et al. [8] and Kamrin and Koval [78], and gray symbols denote the DEM data of the present work. The solid line denotes the fit of (3.1) with $\mu_s = 0.272$ and $b = 1.168$.

previous works [41], we take $k_t/k_n = 1/2$ and $e = 0.1$. Finally, among the interaction parameters, $\mu_{\text{surf}}$ plays the most important role [78]. Exploring the effect of $\mu_{\text{surf}}$ on the flow threshold is beyond the scope of the present work, so we restrict attention to the case of $\mu_{\text{surf}} = 0.4$. The equations of motion for each particle are solved using standard molecular dynamics techniques using the open-source software LAMMPS [79]. For the most part, we restrict the time step to be 0.01 of the binary collision time, $\tau_c = \sqrt{m(\pi^2 + \ln^2 e)/4k_n}$, to ensure stable, accurate simulation results.\(^3\)

3.2.2 Planar shear flow

First, we perform simulations of planar shear flow in order to verify our DEM results against existing data reported in the literature. We consider a configuration consisting of a rectangular region of length $L = 60d$ in the $x$-direction and height $H = 60d$ in the $z$-direction that is filled with a dense collection of 3806 flowing grains and subjected to shearing through the relative motion of two parallel, rough walls, as shown in Fig. 3.2(a).

\(^3\)A larger time step is used for certain DEM simulations of planar shear flow and planar shear flow with gravity to save computation time. The time step is never taken to be greater than 0.1 of $\tau_c$ and has been verified to not affect results.
The dense granular system is generated by allowing grains to sediment under the action of gravity, but gravity is absent in subsequent simulations of planar shear. Each of the two rough walls on top and bottom consists of a thin layer of touching glued grains, which are denoted as black in Fig. 3.2(a), while the flowing grains between the walls are denoted as gray. Regarding wall conditions, the bottom wall is fixed, and the velocity of the top wall in the $x$-direction is specified to be $v_{\text{wall}}$. Following da Cruz et al. [8] and subsequent works [41, 78], the velocity of the top wall in the $z$-direction is not zero — i.e., $H$ is not fixed. Instead, in order to maintain a target wall normal stress of $\sigma_{zz}(z = 0) = -P_{\text{wall}}$, the vertical position of the wall is continuously adjusted so that the value of $H$ evolves through $\dot{H} = (-\sigma_{zz}(z = 0) - P_{\text{wall}})L/g_p$, where $g_p$ is a damping parameter for vertical wall motion. Throughout, we take $g_p = 100\sqrt{m\kappa}$. Periodic boundary conditions are utilized in the $x$-direction.

Next, we extract steady velocity and stress fields from DEM simulations of planar shear flow for a range of wall velocities, $v_{\text{wall}}$, and fixed wall pressure, $P_{\text{wall}}$. To ensure that steady flow is achieved, each simulation of planar shear is first run to a top-wall shear displacement of at least $400H$ Then, we consider 1000 system snapshots uniformly distributed in time over an additional top-wall shear displacement of $250H$. Anticipating that the velocity and stress fields are homogeneous along the $x$-direction, we average along the $x$-direction at discrete $z$-positions for each snapshot. We utilize the spatial averaging technique described by Koval and coworkers [41, 78], which is briefly summarized in Appendix B.1. The instantaneous velocity and stress fields are then arithmetically averaged over all snapshots to obtain steady fields that depend only upon the $z$-coordinate. In all cases of planar shear flow, the steady velocity field $v_x(z)$ is linear with very little wall slip, allowing us to define a corresponding, spatially-constant shear strain-rate $\dot{\gamma} = |dv_x/dz|$. All stress components are spatially constant as well. Moreover, the normal stresses $\sigma_{xx}$ and $\sigma_{zz}$ are approximately equal. Therefore, the shear stress and pressure may be denoted as $\tau = |\sigma_{xz}| = |\sigma_{zx}|$ and $P =$

---

$^4$Experience tells us that flow typically reaches steady state within a top-wall shear displacement of $100H$ after a short transient.
\[ -\sigma_{zz} \approx -\sigma_{xx}, \] respectively, and we may calculate the inertial number \( I = \dot{\gamma}\sqrt{m/P} \) and stress ratio \( \mu = \tau/P \) corresponding to each prescribed wall velocity. The relationship between \( \mu \) and \( I \) extracted from our DEM simulations is plotted in Fig. 3.2(b) as gray symbols, along with the DEM data of da Cruz et al. [8] and Kamrin and Koval [78] for stiff, frictional disks with \( \mu_{\text{surf}} = 0.4 \) as black symbols. The DEM results are consistent, verifying our methodology. The DEM data for two-dimensional granular systems consisting of disks may be fit by a simple Bingham-like functional form of the inertial rheology [8]:

\[ \mu_{\text{loc}}(I) = \mu_s + bI, \] (3.1)

where \( \mu_s \) and \( b \) are dimensionless material parameters. This functional form for \( \mu_{\text{loc}}(I) \) is simpler than the nonlinear form (2.1) of Jop et al. [9] used in Chapter 2 and is suitable under conditions in which \( \mu \) does not increase substantially above \( \mu_s \). The relation (3.1) – using fitted parameter values of \( \mu_s = 0.272 \) and \( b = 1.168 \) – is plotted in Fig. 3.2(b), demonstrating that the linear form (3.1) captures DEM data for homogeneous planar shear.

### 3.3 Granular rheology and the flow threshold

In this section, we discuss the nonlocal granular fluidity model for steady, dense granular flow and its attendant description of the flow threshold. Recall from Chapter 2 that in the NGF model, a positive, scalar field quantity – the granular fluidity – is introduced and denoted as \( g \). Then, instead of relating the stress state to the strain-rate through a single constitutive equation as in the inertial rheology (3.1), the NGF model relates the stress state, the strain-rate, and the granular fluidity through two constitutive equations as follows:

\[ \dot{\gamma} = g\mu, \] (3.2)

\[ t_0 \frac{Dg}{Dt} = A^2 d^2 \frac{\partial^2 g}{\partial x_k \partial x_k} - (\mu_s - \mu)g - b\sqrt{\frac{m}{P}}\mu g^2, \] (3.3)
where $t_0 > 0$ is a constant timescale associated with the dynamics of $g$, $A > 0$ is a constant dimensionless material parameter characterizing nonlocal effects, called the nonlocal amplitude, and the dimensionless constants $\mu_s$ and $b$ are the same as those appearing in the local inertial rheology (3.1). The duel constitutive roles of the granular fluidity become clear in (3.2) and (3.3). First, in (3.2), $g$ operates as a fluidity-like quantity, relating the stress ratio $\mu$ to the consequent shear strain-rate $\dot{\gamma}$, and second, in (3.3), $g$ operates as a nonlocal order parameter governed by a dynamical system. When the flow field is homogeneous, the granular fluidity evolves to the stable, steady, stress-dependent solution of the dynamical system (3.3), which is given by

$$g_{\text{loc}}(\mu, P) = \begin{cases} \sqrt{\frac{P}{m} \left( \frac{\mu - \mu_s}{b\mu} \right)} & \text{if } \mu > \mu_s, \\ 0 & \text{if } \mu \leq \mu_s, \end{cases}$$ (3.4)

and referred to as the local fluidity. When the granular fluidity is given through (3.4) and combined with (3.2), the local inertial rheology (3.1) is recovered, and hence, the NGF model reduces to the inertial rheology for steady, homogeneous flow. However, when flow gradients are present, the Laplacian term in (3.3) introduces an intrinsic length-scale given through the grain size $d$, and the NGF model produces nonlocal predictions.

Several comments on the dynamical relation (3.3) are in order:

1. As discussed in Henann and Kamrin [60], the last two terms in (3.3) arise through the derivative of a coarse-grain Ginzburg-Landau-type free energy. Since these terms then determine the stable, steady solution for $g$ in the absence of flow gradients – i.e., the local fluidity (3.4) – the choices of the Ginzburg-Landau-type free energy and the fitting function for the local inertial rheology are one and the same. Hence, if one were to utilize a different functional form for the inertial rheology than the Bingham-like form (3.1) – as we did in Chapter 2 – it would be necessary to modify these terms in (3.3). Indeed, this is the reason that different forms for the last two terms are adopted in (2.5) and (3.3). In previous work applying the NGF model to dense flows
of spheres down inclines [58], the nonlinear fitting function (2.1) of Jop et al. [9] was used, and hence, the dynamical relation took on the form (2.5). In this chapter, focusing on two-dimensional granular systems of disks, the Bingham-like form of the inertial rheology works well up to a stress ratio of 0.5 (see Fig. 3.2(b)), so we utilize the corresponding dynamical form (3.3), while limiting attention to situations in which the stress ratio remains less than 0.5.

2. The dynamics embodied by (3.3) does not involve bistability, in which two stable, steady-state values of \( g \) exist for some range of \( \mu \). This feature would lead to a non-monotonic local rheology and hysteresis of the predicted flow threshold. There is some experimental evidence for a non-monotonic local rheology in dense flows of spheres [80]; however, non-monotonicity is not observed in our DEM simulations of disks, so we neglect the possibility of this effect in the present work.

3. The time-dependent term appearing in (3.3) is not intended to quantitatively describe the approach to steady state, such as the transient variations in flow resistance that accompany Reynolds dilatancy or the transient effects reported by Ries et al. [71]. However, the model does provide an accurate description of the long-term dynamical behavior – i.e., steady flow – as well as the flow threshold. In these cases, the numerical value of the positive parameter \( \tau_0 \) appearing in (3.3) is irrelevant.

4. The differential relation (3.3) may be reduced to the steady-state-only form under the approximation that deviations of the granular fluidity \( g \) from the local fluidity \( g_{\text{loc}} \) are small. The result of such an approximation – the details of which are discussed in Henann and Kamrin [60] – is

\[
g = g_{\text{loc}} + \xi^2 \frac{\partial^2 g}{\partial x_k \partial x_k} \quad \text{with} \quad \xi(\mu) = \frac{Ad}{\sqrt{|\mu - \mu_s|}},
\]

(3.5)

where \( g_{\text{loc}}(\mu, P) \) is the local fluidity function (3.4) and \( \xi(\mu) \) is the stress-dependent
cooperativity length. The steady-state form of the NGF model may be straightforwardly applied to obtain accurate predictions of non-uniform steady flow fields in a variety of geometric configurations – as illustrated in Chapter 2 in the context of dense heap flows. However, (3.5) cannot capture the size-dependence of the flow threshold. To see this, note that the local fluidity function (3.4) mathematically acts as a source term in (3.5) and is non-zero whenever \( \mu > \mu_s \). Then, when \( \mu \) exceeds \( \mu_s \) at any point in a dense granular medium, (3.5) will predict flowing solutions, regardless of the size of the granular medium. This deficiency arises because the approximation that \( g \) is close to \( g_{loc} \) breaks down as the size of a granular medium decreases. For example, in dense granular flows down an incline, flow arrests in thin layers when \( \mu \) is significantly greater than \( \mu_s \) and hence \( g_{loc} \) is significantly greater than zero. Therefore, to obtain predictions of the size-dependence of the flow threshold, we utilize the primitive, dynamical form of the NGF model (3.3) exclusively throughout the remainder of this chapter.

Next, we discuss how predictions of the flow threshold may be obtained from the NGF model. For the local inertial rheology, the flow threshold is determined by simply comparing the maximum value of the stress ratio \( \mu \) occurring in a flow configuration to the critical value \( \mu_s \). However, for the nonlocal model (3.3), this method of assessing the flow threshold is no longer sufficient. Instead, we reframe the question of whether or not steady flow is possible as whether or not the \( g = 0 \) solution is linearly stable under perturbation. Starting from (3.3) and linearizing about the \( g = 0 \) solution renders the \( g^2 \) term negligible, and we assume a perturbed solution \( \hat{g} \) of the form \( \hat{g}(x,t) = C \exp(\lambda t/t_0)\hat{g}(x) \), where \( \lambda \) is the dimensionless growth rate of the perturbation, \( \hat{g}(x) \) is a time-independent function, \( x \) is the spatial coordinate, and \( C \) is an arbitrary constant. Substituting the perturbed solution \( \hat{g} \) into the linearized form of (3.3) and simplifying, we obtain the following linear differential relation for \( \hat{g} \):

\[
A^2d^2\frac{\partial^2 \hat{g}}{\partial x_k \partial x_k} - (\lambda + \mu_s - \mu) \hat{g} = 0. \tag{3.6}
\]
Then, for a given flow configuration, the field $\mu(x)$ is specified along with appropriate homogeneous boundary conditions for $\dot{g}$, and the growth rate $\lambda$ may be calculated. If $\lambda < 0$, the perturbation decays, and steady flow is not possible. If $\lambda > 0$, the perturbation grows, and steady flow may occur. The flow threshold may be identified as the case in which $\lambda = 0$. In subsequent discussions of the theoretically predicted flow threshold, we denote $\dot{g}$ as $g$ for notational simplicity.

The NGF-model-predicted flow threshold for inclined plane flow has been derived in previous work [58]. Here, we briefly recap the linear perturbation process that will subsequently be applied to the more complex flow configurations in Section 3.4. The $\mu$-field in inclined plane flow is spatially constant and given through the angle of inclination by $\tan \theta$, i.e., $\mu = \tan \theta$. Therefore, (3.6) takes the form of an ordinary differential equation (ODE) with constant coefficients:

$$\frac{d^2 g}{dz^2} + \left( \frac{\tan \theta - \lambda - \mu_s}{A^2d^2} \right) g = 0, \quad (3.7)$$

where $z$ is the distance from the free surface. Anticipating that the quantity $(\tan \theta - \lambda - \mu_s)$ is positive, the solution to (3.7) is

$$g = C_1 \sin \left( \frac{\sqrt{\tan \theta - \lambda - \mu_s}}{Ad} z \right) + C_2 \cos \left( \frac{\sqrt{\tan \theta - \lambda - \mu_s}}{Ad} z \right),$$

where $C_1$ and $C_2$ are arbitrary constants. As discussed in previous work [58], the choice of homogeneous boundary conditions is important. For inclined plane flow, we based this choice on observations of existing DEM flow data of spheres [30]. In particular, in the region near the free surface ($z = 0$), the DEM data of Silbert et al. [30] shows that the strain-rate approximately levels off, implying a zero strain-rate gradient. Accordingly, we enforce that $dg/dz = 0$ at $z = 0$, which requires that $C_1 = 0$. Second, Silbert et al. [30] observed that adjacent to a fully rough boundary, the strain-rate approaches an approximately vanishing state, and hence, we take $g = 0$ at $z = H$. The lowest value of $\tan \theta$ that satisfies this
boundary condition corresponds to

\[
\frac{H}{d} = \frac{\pi A}{2 \sqrt{\tan \theta - \mu_s}}.
\]  

(3.8)

In (3.8), \( \lambda \) has been set to zero, so that (3.8) represents the size-dependent flow threshold for inclined plane flow. For thick layers, the flow threshold approaches the size-independent value \( \tan \theta = \mu_s \); however, for thinner layers, flow ceases at higher inclination angles. In Fig. 3.1(b), the predicted flow threshold (3.8) is compared against Pouliquen’s experimentally determined values using glass beads with a fully rough base, using the parameters for glass beads (\( \mu_s = 0.3819 \) and \( A = 0.48 \)), and the agreement is quite good. To obtain the flow thresholds corresponding to the more complex flow configurations considered in Section 3.4, we apply the same linear perturbation process – albeit involving more complex stress ratio fields. The details of these calculations and the resulting theoretical flow thresholds are given in Section 3.4.

A deeper discussion of the role of fluidity boundary conditions in NGF model predictions of the flow threshold is warranted. In the case of inclined plane flow, it is the choice of a homogeneous Dirichlet fluidity boundary condition at the rough base that leads to predictions of size-dependent strengthening. Indeed, if a homogeneous Neumann condition were employed, a size-independent angle of repose would be predicted. However, as will be shown in Section 3.4, NGF model predictions of size-dependent strengthening do not arise solely due to wall conditions. In a flow configuration with a spatially varying \( \mu \)-field, in which some spatial regions experience \( \mu > \mu_s \) while others experience \( \mu < \mu_s \), the NGF model also predicts size-dependent strengthening, regardless of the choice of wall boundary condition. In such a case, the region experiencing \( \mu < \mu_s \) serves to stabilize the region experiencing \( \mu > \mu_s \) through nonlocal effects, while a local model would simply predict the region experiencing \( \mu > \mu_s \) to flow. The flow configurations considered in Section 3.4 involve both spatially varying \( \mu \)-fields and rough walls. In the DEM simulations reported
in Section 3.4, we are unable to extract clear evidence justifying a homogeneous Dirichlet boundary condition for the fluidity at walls. Therefore, for the sake of simplicity, following our previous work [28, 57, 81], we employ homogeneous Neumann fluidity boundary conditions at walls throughout – both in calculating theoretical flow thresholds and steady flow fields. We note that a similar choice of wall fluidity boundary condition was employed by Chaudhuri et al. [82] in their investigation of vertical chute flow of soft, frictionless disks. In spite of this rather naive choice of fluidity boundary condition, the results of Section 3.4 demonstrate that good agreement between DEM data and NGF model predictions may be obtained, indicating that the specifics of the stress field may play a larger role than wall conditions.

### 3.4 Flow threshold in other configurations

In this section, we present DEM simulation results in three flow configurations – planar shear flow with gravity, annular shear flow, and vertical chute flow – characterizing the size-dependence of the flow threshold in each case. To be clear, in the context of our DEM simulations, the flow threshold refers to the condition for flow cessation and not the condition for flow start-up, which is typically greater than the flow cessation condition and is dependent on the preparation history. In this section, we also compare DEM results with corresponding predictions of the NGF model. Throughout, we use a single set of material parameters $\{\mu_s, b, A\}$ in obtaining NGF model predictions. Based on the fit of the Bingham-like functional form of the inertial rheology (3.1) to DEM data of homogeneous planar shearing (Fig. 3.2(b)), we utilize local parameter values of $\mu_s = 0.272$ and $b = 1.168$. In contrast, the nonlocal amplitude is not obtained by fitting to a single data set – rather, we choose a value of $A = 0.90$ in order to provide the best collective description of all subsequently reported data. We note that this numerical value is similar to the value $A = 0.80$, which was reported by Kamrin and Koval [78] for disks with an inter-particle sliding...
3.4.1 Planar shear flow with gravity

First, we consider planar shear flow with gravity acting orthogonal to the shearing direction. We note that size-dependent strengthening in this configuration was first suggested by Pouliquen and Forterre [45] in the context of their modeling work, but to our knowledge, this effect has not been reported in experiments or DEM simulations. The DEM set-up for this case is shown in Fig. 3.3 (a) and is achieved by introducing a gravitational body

friction coefficient $\mu_{\text{surf}} = 0.4$. 

Figure 3.3: (a) Configuration for two-dimensional DEM simulations of planar shear flow with gravity. (b) The dependence of the stress ratio at the wall $\mu_{\text{wall}}$ on $\tilde{v}_{\text{wall}}$ for loading length-scales $\ell/d = P_{\text{wall}}/\phi \rho_s Gd = 11.75, 23.5, 47$, and $93.5$. (c) Flow threshold locus. (d) Normalized steady velocity fields in the plateau regime ($\tilde{v}_{\text{wall}} \approx 10^{-3}$) for the four loading length-scales in (b). Inset: Steady stress ratio fields corresponding to each case. Throughout, symbols represent the steady-state results of DEM simulations. In (b) and (d), solid lines are the calculated steady results of the NGF model, (3.2) and (3.3). In (c), the solid line is the analytical flow threshold predicted by the NGF model (3.12). In the inset of (d), the solid lines are the anticipated $\mu$-fields (3.9) used as input in calculations involving the NGF model.
force along the \( z \)-direction to the configuration used in planar shear flow, described in Section 3.2.2. The parallel, rough walls are separated by a distance \( H = 60d \), and the top wall moves in the \( x \)-direction with a velocity \( v_{\text{wall}} \), while the bottom wall remains fixed. The top wall imposes a compressive normal stress \( P_{\text{wall}} \) on the granular material, using the control procedure described in Section 3.2.2 and the gravitational body force is \( \phi \rho_s G \), where \( \phi \) is the mean solid area fraction and \( G \) is the acceleration of gravity. Periodic boundary conditions are employed along the \( x \)-direction, and the length of the region in the \( x \)-direction is \( L = 60d \).

The expected stress field in this flow configuration may be deduced from a quasi-static force balance. As in planar shear flow without gravity, the shear stress is spatially constant and given by the shear stress imparted by the moving wall – i.e., \( \tau(z) = |\sigma_{xz}(z)| = |\sigma_{zx}(z)| = \tau_{\text{wall}} \). The pressure field is a combination of the prescribed wall pressure \( P_{\text{wall}} \) and the gravitational pressure gradient, so that \( P(z) = -\sigma_{zz}(z) = P_{\text{wall}} + \phi \rho_s G z \). As in planar shear flow, we assume that \( \sigma_{xx}(z) \approx \sigma_{zz}(z) \), which is consistent with the results of our DEM simulations. Therefore, the stress ratio field in planar shear flow with gravity varies as

\[
\mu(z) = \frac{\tau(z)}{P(z)} = \frac{\mu_{\text{wall}}}{1 + z/\ell},
\]

where \( \mu_{\text{wall}} = \tau_{\text{wall}}/P_{\text{wall}} \) is the maximum value of \( \mu \), occurring at the wall \((z = 0)\), and \( \ell = P_{\text{wall}}/\phi \rho_s G \) is the loading length-scale, which is defined as the ratio of the wall pressure to the gravitational body force and is distinct from the dimensions \( H \) and \( L \). Importantly, since the loading length-scale \( \ell \) is the only length-scale appearing in the stress ratio field \((3.9)\), \( \ell \) – rather than the dimensions \( H \) or \( L \) – is the relevant length-scale that characterizes the system size in this problem. The loading length-scale \( \ell \) may be interpreted as the distance beneath the top wall at which the pressure due to gravity \( \phi \rho_s G \ell \) is equal to the pressure applied by the top wall \( P_{\text{wall}} \) – i.e., \( P(z = \ell) = 2P_{\text{wall}} \). We have verified that the dimensions \( H = 60d \) and \( L = 60d \) are sufficiently large so that they do not affect the subsequently
We run DEM simulations of planar shear flow with gravity for different values of the top-wall speed \( v_{\text{wall}} \) and loading length-scale \( \ell \). Each DEM simulation is run to steady state through a top-wall shear displacement of at least \( 5500d \), and the steady fields \( v_x(z) \), \( \tau(z) \), and \( P(z) \) are calculated using 2000 system snapshots – evenly spaced over an additional top-wall shear displacement of at least \( 5500d \) – as described in Appendix B.1. In each case, we verify that the resulting shear stress field is indeed constant – thereby extracting the corresponding value of \( \tau_{\text{wall}} \) – and that the pressure field matches the intended dependence \( P(z) = P_{\text{wall}} + \phi \rho_s Gz \). In presenting results, we utilize a dimensionless wall velocity \( \tilde{v}_{\text{wall}} = (v_{\text{wall}}/\ell) \sqrt{m/P_{\text{wall}}} \), in which \( v_{\text{wall}} \) is non-dimensionalized through the loading length-scale and the microscopic time-scale associated with particle motion. First, we probe the dependence of the stress ratio at the wall \( \mu_{\text{wall}} = \tau_{\text{wall}}/P_{\text{wall}} \) on \( \tilde{v}_{\text{wall}} \) for loading length-scales \( \ell/d = 11.75, 23.5, 47, \) and \( 93.5 \), which is plotted as symbols in Fig. 3.3(b). For sufficiently high wall speed – i.e., \( \tilde{v}_{\text{wall}} \gtrsim 3 \times 10^{-2} \) – the relationship between \( \mu_{\text{wall}} \) and \( \tilde{v}_{\text{wall}} \) is size-independent, indicating that the response is dominated by local, inertial effects. However, as the wall speed is decreased, a rate-independent plateau emerges, which is dependent on the system-size \( \ell/d \). Therefore, for a given \( \ell/d \), steady flow is not possible for \( \mu_{\text{wall}} \) less than the plateau value, enabling the construction of a phase diagram of flowing and non-flowing states. As shown in Fig. 3.3(c), we create a phase diagram with \( \ell/d \) on the vertical axis and \( \mu_{\text{wall}} \) on the horizontal axis. Then, the DEM-calculated flow threshold locus is plotted as symbols on the phase diagram – in which each point consists of a given \( \ell/d \) and the corresponding plateau value of \( \mu_{\text{wall}} \). Steady flow is possible for combinations of \( \ell/d \) and \( \mu_{\text{wall}} \) to the right of the flow threshold locus, while steady flow cannot occur for combinations to the left of the locus. For a large system-size, the flow threshold approaches the size-independent value \( \mu_s \); however, as \( \ell/d \) decreases the flow threshold increases.

We have also numerically computed corresponding steady solutions of the NGF model,
Model predictions of steady velocity fields are calculated for a given combination of $\ell/d$ and $\mu_{\text{wall}}$, by evolving (3.3) to steady state, using finite differences in MATLAB with $\mu$-field given through (3.9), a very fine spatial resolution $\Delta z \ll d$, and the solution of (3.5) as the initial guess. The calculated relationships between the wall stress ratio $\mu_{\text{wall}}$ and the dimensionless wall speed $\tilde{v}_{\text{wall}}$ are plotted as solid lines in Fig. 3.3(b) for $\ell/d = 11.75, 23.5, 47,$ and 93.5. The NGF model quantitatively captures both the size-independent but rate-dependent regime observed in DEM simulations at sufficiently high wall speed and the size-dependent but rate-independent plateau regime – an observation that may be understood in terms of the dynamical relation (3.3) as follows. At sufficiently high wall speed, the Laplacian term in (3.3) contributes negligibly, yielding size-independent model predictions. Consequently, the parameters $\mu_s$ and $b$ – but not $A$ – set the model predictions in the rate-dependent regime. In contrast, for sufficiently slow flows, the $g^2$ term plays a negligible role, rendering the dynamical relation (3.3) linear in $g$ which leads to rate-independent model predictions. The parameters $\mu_s$ and $A$ – but not $b$ – determine NGF model predictions in the rate-independent regime.

The plateau value of $\mu_{\text{wall}}$ calculated using the NGF model for a given value of $\ell/d$ then represents a point on the predicted flow threshold locus. Instead of constructing the locus using discrete points determined in this way, we have calculated the analytical flow threshold predicted by the NGF model for planar shear flow with gravity using the linear perturbation procedure described in Section 3.3. We define a dimensionless transformed coordinate $\tilde{z}$ and a positive, dimensionless constant $\alpha$ as

$$\tilde{z} = 2\sqrt{\lambda + \mu_s (z + \ell)} = \frac{2\sqrt{\lambda + \mu_s (z + \ell)}}{Ad}$$

$$\alpha = \frac{2\sqrt{\lambda + \mu_s (z + \ell)}}{2\sqrt{\lambda + \mu_s Ad}} = \frac{\mu_{\text{wall}}}{2\sqrt{\lambda + \mu_s Ad}}.$$

Then, upon substituting the $\mu$-field for planar shear flow with gravity (3.9) into (3.6), the
resulting linear ODE for \( g(\tilde{z}) \) is

\[
\frac{d^2 g}{d\tilde{z}^2} + \left( -\frac{1}{4} + \frac{\alpha}{\tilde{z}} \right) g = 0. \quad (3.11)
\]

The solution of (3.11) is

\[ g = C_1 M_{\alpha,1/2}(\tilde{z}) + C_2 W_{\alpha,1/2}(\tilde{z}), \]

where \( M_{\alpha,1/2}(\tilde{z}) \) and \( W_{\alpha,1/2}(\tilde{z}) \) are Whittaker functions, and \( C_1 \) and \( C_2 \) are constants. The homogeneous boundary conditions consist of a Neumann condition at the moving wall, \( \frac{dg}{d\tilde{z}}|_{\tilde{z}=0} = 0 \), and the far-field boundary condition, \( \lim_{\tilde{z} \to \infty} g = 0 \). Since the function \( M_{\alpha,1/2}(\tilde{z}) \) diverges as \( \tilde{z} \to \infty \), while \( W_{\alpha,1/2}(\tilde{z}) \to 0 \), the far-field boundary condition requires that \( C_1 = 0 \). Then, applying the wall boundary condition, making use of the identity \( W'_{\alpha,1/2}(\tilde{z}) = ((\tilde{z} - 2\alpha)W_{\alpha,1/2}(\tilde{z}) - 2W_{\alpha+1,1/2}(\tilde{z}))/2\tilde{z} \), and simplifying, we obtain

\[
\left( \sqrt{\mu_s} \frac{\ell}{Ad} - \alpha \right) W_{\alpha,1/2} \left( 2\sqrt{\mu_s} \frac{\ell}{Ad} \right) - W_{\alpha+1,1/2} \left( 2\sqrt{\mu_s} \frac{\ell}{Ad} \right) = 0 \quad \text{with} \quad \alpha = \frac{\mu_{\text{wall}}}{2\sqrt{\mu_s} Ad}. \quad (3.12)
\]

In the above expression, we have set \( \lambda \) to the threshold value of \( \lambda = 0 \), so that (3.12) represents the size-dependent flow threshold for planar shear with gravity. For a given value of the dimensionless system size \( \ell/d \) and the material parameters \( \mu_s \) and \( A \), the smallest, positive value of \( \mu_{\text{wall}} \) that satisfies the transcendental equation (3.12) gives the flow threshold. The analytical flow threshold (3.12) is plotted as a solid line in Fig. 3.3(c) – displaying a favorable quantitative comparison with the DEM data.

Finally, we compare steady velocity fields extracted from DEM simulations to corresponding NGF model predictions. Steady normalized velocity fields \( v_x(z)/v_{\text{wall}} \) in the plateau regime (\( v_{\text{wall}} \approx 10^{-3} \)) for loading length-scales \( \ell/d = 11.75, 23.5, 47, \) and 93.5 are shown in Fig. 3.3(d) with symbols denoting DEM data and solid lines representing NGF model predictions. In the inset of Fig. 3.3(d), symbols denote the corresponding normalized stress ratio fields \( \mu(z)/\mu_{\text{wall}} \) measured in the DEM simulations, and solid lines
represent the anticipated stress ratio fields used as input in calculations involving the NGF model, confirming that the intended stress fields are achieved in the DEM simulations. Overall, the NGF model is able to quantitatively capture the salient aspects of the flow fields in planar shear flow with gravity over a range of loading length-scales. Importantly, the nonlocal amplitude $A$ is the operative material parameter that determines NGF model predictions of steady flow fields in the plateau regime, and using a single numerical value of $A$, the NGF model simultaneously captures DEM data of both the size-dependence of the flow threshold and steady flow fields.

3.4.2 Annular shear flow

Next, we consider annular shear flow – the DEM set-up for which is shown in Fig. 3.4(a) with inner radius $R$ and outer radius $R_o$. For the most part, the details of our DEM simulations of annular shear flow follow the procedures of Koval and coworkers [41, 78]. The walls in our DEM simulations of annular shear flow consist of rings of glued grains of diameter $2d$ and the inner radius $R$ corresponds to the radial position of the outermost points of the inner wall grains. At the inner wall, we prescribe the circumferential wall velocity $v_{\text{wall}}$, and the radial position of the inner wall grains is fixed. While the outer wall does not rotate, the value of $R_o$ fluctuates slightly so as to impose a prescribed radial compressive normal stress $P_{\text{wall}}$ on the granular material, using a control procedure analogous to that used in Section 3.2.2 and described by Koval et al. [41]. We do not utilize periodic boundary conditions, instead modeling the full annular shear cell, as shown in Fig. 3.4(a) for the case of $R/d = 26$. In total, we consider inner wall radii of $R/d = 11, 26, 51,$ and 101. Throughout, we take the outer radius to be sufficiently large so that the value of $R_o$ does not affect the subsequently reported results -- $R_o = 2R$ for $R/d = 25, 51,$ and 101 and

---

5Rough walls consisting of glued grains of diameter $2d$ were also used in the annular shear flow simulations of Kamrin and Koval [78]. We utilize this type of rough wall for our annular shear flow simulations rather than the rough walls described in Section 3.2.2 in order to more easily construct the annular DEM configuration.
Analogous to planar shear with gravity, we may deduce the steady stress field from quasi-static force and moment balances. The moment balance gives the shear stress field to be $\tau(r) = |\sigma_{r\theta}(r)| = |\sigma_{\theta r}(r)| = \tau_{\text{wall}}(R/r)^2$, where $r$ is the radial coordinate and $\tau_{\text{wall}}$ is the inner wall shear stress, and the radial force balance gives that $P(r) = -\sigma_{rr}(r) = P_{\text{wall}}$ is spatially constant. Again, we assume that the normal stresses are equal – i.e., $\sigma_{\theta\theta} \approx \sigma_{rr}$ – which is consistent with DEM simulation results. Therefore, for annular shear flow, the

$$R_0 = 4R$$

for $R/d = 11$. The DEM configurations for $R/d = 11, 26, 51, 101$ contain 4640, 5715, 23900, and 97696 flowing grains, respectively.
stress ratio field varies as
\[ \mu(r) = \frac{\tau(r)}{P(r)} = \mu_{\text{wall}} \left( \frac{R}{r} \right)^2, \]  
where \( \mu_{\text{wall}} = \frac{\tau_{\text{wall}}}{P_{\text{wall}}} \) is the maximum value of \( \mu \), occurring at the inner wall \((r = R)\).

Our discussion of simulation results for annular shear flow mirrors that of Section 3.4.1 for planar shear flow with gravity. We run DEM simulations for different values of the inner wall speed \( v_{\text{wall}} \) and radius \( R \). Each simulation is first run to steady state through an inner-wall tangential displacement of at least \( 48d \) and the steady fields \( v_\theta(r) \), \( \tau(r) \), and \( P(r) \) are then extracted using 1000 system snapshots, which are evenly spaced over an additional inner-wall tangential displacement of an equal amount as in the preceding step. Further, \( \tau_{\text{wall}} \) is measured by way of the average torque applied to the inner wall at steady state. First, we explore the dependence of the inner wall stress ratio \( \mu_{\text{wall}} \) on \( \tilde{v}_{\text{wall}} = (v_{\text{wall}}/R)\sqrt{m/P_{\text{wall}}} \) in DEM simulations for \( R/d = 26, 51, \) and 101, which is plotted as symbols in Fig. 3.4(b). Again, a transition is observed from a rate-dependent but size-independent regime at sufficiently high wall speed \( \tilde{v}_{\text{wall}} \gtrsim 10^{-2} \) to a size-dependent plateau regime as \( \tilde{v}_{\text{wall}} \) is decreased. Here, we have restricted attention to a slightly lower range of \( \tilde{v}_{\text{wall}} \) than considered in Section 3.4.1 to ensure that centripetal acceleration plays no role in our DEM simulations – a point which is verified by checking that the normal stress \( \sigma_{rr} \) is spatially constant. A phase diagram of flowing and non-flowing states for annular shear flow is shown in Fig. 3.4(c), in which pairs of \( R/d \) and the corresponding plateau value of \( \mu_{\text{wall}} \) are plotted as symbols and denote the DEM-calculated flow threshold locus. Again, we observe strengthening as the system-size \( R/d \) is reduced.

Steady-state predictions of the NGF model are numerically calculated for given combinations of \( R/d \) and \( \mu_{\text{wall}} \) as described in Section 3.4.1 except with \( \mu \)-field given through (3.13). The calculated relationships between \( \mu_{\text{wall}} \) and \( \tilde{v}_{\text{wall}} \) are plotted as solid lines in

\footnote{Koval and coworkers \cite{41, 78} report that transients fully subside after an inner-wall tangential displacement of approximately \( 50d \) in their simulations of annular shear flow and conservatively adopt an inner-wall displacement of \( 100d \) as their steady-state condition. Our observation of transients is similar, and for efficiency – since we simulate the full annular shear cell rather than an angular section – we adopt a steady-state condition of \( 48d \) for the inner-wall displacement.}
Fig. 3.4(b) for $R/d = 26, 51, \text{ and } 101$, demonstrating good quantitative agreement with DEM data and – most importantly – displaying a size-dependent plateau value of $\mu_{\text{wall}}$. As in Section 3.4.1, we calculate the theoretical flow threshold locus for annular shear flow via the linear perturbation procedure described in Section 3.3. Substituting the $\mu$-field (3.13) into (3.6), defining a dimensionless transformed coordinate $\tilde{r}$ and a positive, dimensionless constant $\alpha$ as

$$\tilde{r} = \sqrt{\lambda + \mu_s} \frac{r}{Ad} \quad \text{and} \quad \alpha = \sqrt{\mu_{\text{wall}}} \frac{R}{Ad},$$

(3.14)

and simplifying, we obtain the following linear ODE for $g(\tilde{r})$:

$$\tilde{r}^2 \frac{d^2 g}{d\tilde{r}^2} + \tilde{r} \frac{dg}{d\tilde{r}} - (\tilde{r}^2 - \alpha^2) g = 0.$$

(3.15)

The solution of (3.15) is $g = C_1 I_{i\alpha}(\tilde{r}) + C_2 K_{i\alpha}(\tilde{r})$, where $I_{i\alpha}(\tilde{r})$ and $K_{i\alpha}(\tilde{r})$ are the modified Bessel functions of the first and second kind of purely imaginary order, and $C_1$ and $C_2$ are constants. We consider the following homogeneous boundary conditions: a Neumann condition at the inner wall, $dg/dr|_{r=R} = 0$, and the far-field condition, $\lim_{r \to \infty} g = 0$. For $\tilde{r}$ and $\alpha$ positive, the function $I_{i\alpha}(\tilde{r})$ is complex-valued, and its real part diverges as $\tilde{r} \to \infty$. In contrast, $K_{i\alpha}(\tilde{r})$ is real-valued for $\tilde{r}$ and $\alpha$ positive, and $K_{i\alpha}(\tilde{r}) \to 0$ as $\tilde{r} \to \infty$. Therefore, the far-field boundary condition requires that $C_1 = 0$. Then, applying the wall boundary condition, setting $\lambda = 0$, and simplifying leads to the size-dependent flow threshold for annular shear flow:

$$K'_{i\alpha} \left( \sqrt{\mu_s} \frac{R}{Ad} \right) = 0 \quad \text{with} \quad \alpha = \sqrt{\mu_{\text{wall}}} \frac{R}{Ad}. \quad (3.16)$$

For a given value of the dimensionless inner wall radius $R/d$ and the material parameters $\mu_s$ and $A$, the smallest, positive value of $\mu_{\text{wall}}$ that satisfies (3.16) gives the flow threshold. The theoretical flow threshold locus (3.16) is plotted as a solid line in Fig. 3.4(c), showing that the NGF model captures the size-dependent flow threshold in this flow configuration.
Figure 3.5: (a) Configuration for two-dimensional DEM simulations of vertical chute flow for the case of $W/d = 60$. (b) Flow threshold locus. Symbols represent upper and lower bound estimates of the flow threshold based on the results of DEM simulations, and the solid line is the analytical flow threshold predicted by the NGF model (3.19).

Lastly, we compare DEM data and NGF model predictions of steady velocity fields. Steady normalized velocity fields $v_\theta(r)/v_{\text{wall}}$ in the plateau regime ($\bar{v}_{\text{wall}} \approx 10^{-4}$) for inner wall radii $R/d = 26, 51,$ and $101$ are shown in Fig. 3.4(d) with symbols denoting DEM data and solid lines representing NGF model predictions. Corresponding steady normalized stress ratio fields $\mu(r)/\mu_{\text{wall}}$ are shown in the inset of Fig. 3.4(d), confirming that the $\mu$-fields measured from DEM data are consistent with the anticipated stress ratio fields (3.13). The NGF model quantitatively captures both steady flow fields and the size-dependence of the flow threshold in annular shear flow – while using the same set of material parameters as in planar shear flow with gravity.

### 3.4.3 Vertical chute flow

Finally, we consider vertical chute flow. The size-dependence of the flow threshold in this configuration was first explored by Chaudhuri et al. [82] for a simulated, two-dimensional system of soft, frictionless particles. Here, we perform an analogous analysis for our system of stiff, frictional disks. Our DEM set-up is shown in Fig. 3.5(a), which is generated by first creating a dense granular system between two parallel, rough walls as described for planar shear in Section 3.2.2 and then rotating the system clockwise by $90^\circ$ and applying
a gravitational body force along the \(z\)-direction. The rough walls – consisting of layers of glued grains as in the planar shear flow simulations of Section [3.2.2] – are separated by a distance denoted by \(W\), which is varied in our simulations. The left vertical wall is fixed, and the right vertical wall is fixed in the \(z\)-direction but can move slightly in the \(x\)-direction so as to impose a compressive normal stress \(P_{\text{wall}}\) on the granular material, using the control procedure described in Section [3.2.2]. Periodic boundary conditions are prescribed along the \(z\)-direction. In all cases, the length of the vertical chute \(L\) is taken to be \(60d\), which is in a range that does not affect DEM results.\(^7\) We consider nominal chute widths of \(W/d = 10, 20, 30, 40,\) and 60 – however, these values do vary slightly during flow – and the DEM configurations contain 633, 1270, 1900, 2539, and 3806 flowing grains, respectively.

From a quasi-static force balance, we expect the shear stress field to be
\[
\tau(x) = |\sigma_{xz}(x)| = |\sigma_{zx}(x)| = \phi \rho_s G |x|,
\]
where \(x\) is measured from the centerline of the chute, and the pressure field to be
\[
P(x) = -\sigma_{xx}(x) = P_{\text{wall}}.\]
Again, we assume that the normal stresses are equal – i.e., \(\sigma_{zz} \approx \sigma_{xx}\) – and verify this assumption against the DEM results. Therefore, for vertical chute flow, the \(\mu\)-field is
\[
\mu(x) = \mu_{\text{wall}} \left( \frac{|x|}{W/2} \right),
\]
(3.17)
where \(\mu_{\text{wall}} = \phi \rho_s GW/2P_{\text{wall}}\) is the maximum value of \(\mu\), occurring at the walls \((x = \pm W/2)\).

Since vertical chute flow is gravity-driven – while planar shear flow with gravity and annular shear flow are boundary-driven – our process for determining the flow threshold from DEM simulations is different than previously described. In boundary-driven flow, we specify arbitrarily-low wall velocities and extract the flow threshold from the steady-state plateau forces applied to the wall. In contrast, for gravity-driven flow, we consider various conditions – namely, combinations of \(W/d\) and \(\mu_{\text{wall}}\) – and determine whether steady flow

\(^7\)If the vertical chute is taken to be too long, alternating dense and sparse regions will develop along the chute. This is because the procedure employed to control the pressure cannot account for variations along the length of the vertical chute due to the rigid nature of the walls. We have verified that our chute length \(L\) is sufficiently short so that this issue does not arise while also being sufficiently long so that the reported results do not depend upon \(L\).
may be sustained, and in this way, the flow threshold is bounded. Our process is as follows. Motivated by the methodology of Weinhart et al. \cite{31} for assessing flow arrest in DEM simulations of inclined plane flow, we utilize a criteria based on the kinetic energy. First, for a given chute width $W/d$, a sufficiently large value of $\mu_{\text{wall}}$ is applied so that steady flow is attained. Next, $\mu_{\text{wall}}$ is decreased to a target value – in practice, this is achieved by decreasing the acceleration of gravity $G$ – and the system is allowed to reach steady state over a time period of $19470\sqrt{m/P_{\text{wall}}}$. We confirm that the $\mu$-fields measured from steady-state DEM data are consistent with the intended $\mu$-fields (3.17). Then, the mean kinetic energy per flowing grain as a function of time – denoted as $E_{\text{kin}}(t)$ – is extracted from 5000 system snapshots distributed evenly over an additional time period of $19470\sqrt{m/P_{\text{wall}}}$ after reaching steady state. For values of $\mu_{\text{wall}}$ in which the arithmetic average of the kinetic energy $\langle E_{\text{kin}}(t) \rangle$ is greater than $10^{-2}P_{\text{wall}}d^2$\footnote{Since $k_n = 10^4P_{\text{wall}}$ in our simulations, the normalization factor $P_{\text{wall}}d^2$ is related to the elastic potential energy scale, as in Weinhart et al. \cite{31}.}, flow is continuous, and $E_{\text{kin}}(t)$ is nearly time-independent with fluctuations – defined as $(\langle (E_{\text{kin}}(t) - \langle E_{\text{kin}}(t) \rangle)^2 \rangle)^{1/2}$ – smaller than $\langle E_{\text{kin}}(t) \rangle$. When $\mu_{\text{wall}}$ is decreased to a value for which $\langle E_{\text{kin}}(t) \rangle = 10^{-2}P_{\text{wall}}d^2$, fluctuations increase to be roughly equal to $\langle E_{\text{kin}}(t) \rangle$, and accordingly, we identify this condition and the corresponding value of $\mu_{\text{wall}}$ as the upper bound of the flow threshold for a given $W/d$. As $\mu_{\text{wall}}$ is further decreased, flow becomes intermittent, and kinetic energy fluctuations further increase. In this intermittent regime, it is important to acknowledge the effect that the wall damping parameter $g_p$ has on flow. If $g_p$ is too low ($g_p/\sqrt{mk_n} \lesssim 1$), wall motion is underdamped, and the associated wall oscillations prevent flow from ceasing, even when $\mu_{\text{wall}}$ is arbitrarily small. If $g_p$ is too high ($g_p/\sqrt{mk_n} \gtrsim 10^4$), wall motion is overdamped, and the target wall pressure $P_{\text{wall}}$ is not achieved. We find that for our choice of $g_p/\sqrt{mk_n} = 100$, static states may be achieved while maintaining the target wall pressure. That said, using this value of $g_p$, at low values of $\mu_{\text{wall}}$, wall motion can still induce isolated, infrequent grain rearrangements that are not associated with steady flow but do contribute to the kinetic energy. To remove this effect, we median filter the measured kinetic energy
data $E_{\text{kin}}(t)$ for values of $\mu_{\text{wall}}$ in the intermittent regime prior to arithmetically averaging the kinetic energy data over time. When the average value of the filtered kinetic energy data decreases to a very low value of $10^{-7}P_{\text{wall}}d^2$ we deem flow to have ceased and denote the corresponding value of $\mu_{\text{wall}}$ as the lower bound of the flow threshold.

Once upper and lower bounds of the flow threshold have been determined, we may construct a phase diagram of flowing and non-flowing states for vertical chute flow, which is shown in Fig. 3.5(b). For a given $W/d$, the $\times$-symbols denote the upper and lower bounds determined as described in the preceding paragraph, and the range of $\mu_{\text{wall}}$ between the symbols corresponds to the intermediate regime of intermittent flow and is denoted by a dotted line. While the exact value of the chute width varies in our simulations, we find that the differences between actual values of $W$ near the flow threshold and the corresponding nominal values are less than one grain diameter in all cases, so the values of $W/d$ appearing in Fig. 3.5(b) correspond to the nominal values. Due to the presence of the intermittent regime, our determination of the flow threshold in vertical chute flow is less precise than for the flow configurations considered in Sections 3.4.1 and 3.4.2, however, the increase of the measured flow threshold with decreasing system size remains clear.

To calculate the theoretical flow threshold locus predicted by the NGF model for vertical chute flow, we substitute the $\mu$-field (3.17) into (3.6) to obtain

$$\frac{d^2 g}{dx^2} - \ddot{x}g = 0 \quad \text{where} \quad \ddot{x} = \frac{\lambda + \mu_s - \mu_{\text{wall}}x/(W/2)}{(2Ad\mu_{\text{wall}}/W)^{2/3}}$$

is a dimensionless transformed coordinate. The solution of (3.18) is $g = C_1 \text{Ai}(\ddot{x}) + C_2 \text{Bi}(\ddot{x})$, where $\text{Ai}(\ddot{x})$ and $\text{Bi}(\ddot{x})$ are the Airy functions of the first and second kind, and $C_1$ and $C_2$ are constants. The homogeneous boundary conditions consist of the symmetry condition at $x = 0$, $dg/dx|_{x=0} = 0$, and a homogeneous Neumann condition at the wall, $dg/dx|_{x=W/2} = 0$. Enforcing the boundary conditions and setting $\lambda = 0$ yields the size-dependent flow
threshold for vertical chute flow:

\[
A_i' \left( \frac{\mu_s}{(2Ad\mu_{wall}/W)^{2/3}} \right) Bi' \left( \frac{\mu_s - \mu_{wall}}{(2Ad\mu_{wall}/W)^{2/3}} \right) - Bi' \left( \frac{\mu_s}{(2Ad\mu_{wall}/W)^{2/3}} \right) A_i' \left( \frac{\mu_s - \mu_{wall}}{(2Ad\mu_{wall}/W)^{2/3}} \right) = 0. \tag{3.19}
\]

For a given value of the dimensionless chute width \( W/d \) and the material parameters \( \mu_s \) and \( A \), the smallest, positive value of \( \mu_{wall} \) that satisfies (3.19) gives the flow threshold. The theoretical flow threshold locus (3.19) is plotted as a solid line in Fig. 3.5(b), using the same material parameters \( \mu_s \) and \( A \) as in Sections 3.4.1 and 3.4.2. The theoretical flow threshold locus does a reasonably good job of quantitatively capturing the DEM data for vertical chute flow.

### 3.5 Concluding remarks

In this chapter, we have studied the size-dependence of the flow threshold in three different dense granular flow configurations – (1) planar shear flow with gravity, (2) annular shear flow, and (3) vertical chute flow. Importantly, the flow threshold measured in DEM simulations shows substantial size-dependence across all configurations – the details of which are affected by the form of the stress field. We have also applied the NGF model to all three flow configurations to obtain predictions of both the flow threshold and steady flow fields. Notably, we have obtained analytical solutions for the predicted size-dependent flow threshold in all three cases. The theory – using a single set of material parameters – predicts size-dependent flow thresholds that match DEM data rather well in all cases. Further, the theory simultaneously predicts steady flow fields that are quantitatively consistent with corresponding DEM data.

For illustrative purposes, a comparison of the analytical flow thresholds predicted by the NGF model for all four flow configurations discussed in this chapter – inclined plane...
flow (3.8), planar shear flow with gravity (3.12), annular shear flow (3.16), and vertical chute flow (3.19) – is plotted in Fig. 3.6 with the appropriate length-scale on the vertical axis and the maximum value of $\mu$ associated with the flow configuration on the horizontal axis. Notably, size-dependent strengthening in all three configurations considered in Section 3.4 is significantly greater than the strengthening predicted for inclined plane flow. Recall that the strengthening predicted by the theoretical flow threshold for inclined plane flow is entirely due to boundary effects, since the $\mu$-field is spatially constant, while the additional strengthening associated with the other three theoretical flow thresholds is due to the spatial-dependence of the stress field, rather than boundary effects. This observation illustrates that the precise nature of the $\mu$-field has a crucial effect on the resulting flow threshold and must be accounted for when considering other size-sensitive flow stoppage phenomena.

As a final comment, providing physical justification for fluidity boundary conditions at walls remains an open issue. In the present work, our choice of a homogeneous Neumann condition was based on pragmatic grounds – since a homogeneous Dirichlet fluidity boundary condition was not directly observed in our DEM simulations – and past experience – which has shown that such a boundary condition enables an excellent description...
of experiments of split-bottom flow [28] and chute flow [81]. In spite of the lack of a physical underpinning for this choice, the favorable agreement between the flow thresholds measured in DEM simulations and the corresponding analytical flow thresholds predicted by the NGF model provides support for this choice of fluidity boundary condition. From a broader perspective, the issue of specifying non-standard boundary conditions arises in virtually all nonlocal constitutive approaches [46, 54, 55, 82], and motivating the choice of these boundary conditions from a physical perspective remains an open challenge. In the context of nonlocal fluidity models, some recent progress has been made on this point for dense emulsions [83], and future work of this type is needed to develop a clearer microscopic understanding of granular fluidity boundary conditions.
Chapter 4

Modeling shear-rate-gradient-driven and pressure-gradient-driven size-segregation in dense, bidisperse granular flows

Note: A version of this chapter is being prepared for submission to the Journal of Fluid Mechanics. Data and figures have been used with all co-authors’ consent.


4.1 Introduction

The preceding chapters focused on quasi-monodisperse granular systems, in which all grains were approximately the same size. However, most dense granular systems occurring in nature and industry are non-monodisperse – i.e., mixtures consisting of particles of disparate sizes. In non-monodisperse granular systems, it is widely appreciated that the
constituent grains segregate based on size and form complex patterns during flow [18, 84-92]. In geophysics, granular size segregation can manifest in landslides and debris flows, in which more damage is done by the larger grains that segregate to the top of the flow, while in industry, size-segregation can be an undesirable effect when blending granular constituents of various sizes is a necessary processing step.

Granular size-segregation has been repeatedly observed in experiments in the literature. For example, in Thornton et al. [93] for an initially well-mixed system of grains of two different sizes – which we will henceforth refer to as a bidisperse system – flowing down an inclined plane, larger particles segregate to the surface of the flowing layer while smaller ones sink to the bottom. When driving similar bidisperse mixtures in a rotating drum, Gray and Thornton [90] observed small grains segregating to form stripes. As a final example, in split-bottom cell experiments by Hill and Fan [91], not only do the larger particles segregate to the top, but they also segregate towards more rapidly shearing regions.

In terms of the mechanisms of size-segregation in dense granular flows, the current understanding is that there are two driving forces. The first is pressure-gradients – most commonly induced by gravity. In pressure-gradient-driven size-segregation, small particles move more readily through the interstitial space that opens and closes during flow through a process often referred to as “kinetic sieving,” leading to a system stratified along the direction of pressure gradients [90, 94-96]. While pressure-gradient-driven segregation has been the focus of significant study, grains can also segregate in inhomogeneous flows along directions orthogonal to gravitationally-induced pressure gradients [91, 92, 97], driven instead by gradients in shear-strain-rate. As an example, this mechanism has been observed in the aforementioned split-bottom cell experiments of Hill and Fan [91], in which large grains segregate towards shear bands. Shear-strain-rate-gradient-driven segregation has received comparatively less attention and is thus less well understood.

Due to the complexity of coupled flow and segregation patterns, developing a general, predictive, continuum model for granular size-segregation is an open challenge. Although
much invaluable progress has been made over the recent decades [18, 90, 94–98], no ex-
isting models fully account for both segregation dynamics and flow rheology in a self-
contained manner. Instead, they all require some flow field quantity, such as velocity or
stress fluctuation field, to be measured first from experiments or DEM simulations and
then used as model input. A full mechanical continuum model capable of predicting both
the flow fields and the evolution of segregation, based solely on the geometry of the flow
configuration, applied loads, and boundary/initial conditions, is still missing.

The main reason for the incompleteness of current models is the lack of a dense granular
flow rheology theory, which has recently been addressed by the nonlocal granular fluidity
(NGF) model presented in [27, 28, 32, 57, 81] and discussed in the previous chapters.
Thus, our overarching aim is to formulate and validate a predictive continuum theory for
simultaneous flow and size-segregation in dense granular systems by integrating the NGF
model with a phenomenological size-segregation model. This is a broad goal, and in this
work, we narrow our focus to a set of simpler quasi-one-dimensional flow configurations.
In most real-world flows, both the pressure-gradient-driven and shear-strain-rate-gradient-
driven segregation mechanisms are present, making it difficult to disentangle them. There-
fore, our plan is to isolate and examine the shear-strain-rate-gradient-driven mechanism
first before integrating it with the pressure-gradient-driven mechanism and incorporating
both mechanisms into a general, continuum size-segregation model. Specifically, we first
study the shear-strain-rate-gradient-driven segregation by considering flow of dense, bidis-
perse two-dimensional disks in two flow configurations – vertical chute flow and annular
shear flow – in which pressure is constant throughout and no hydrostatic pressure gradients
are present. Therefore shear-strain-rate-gradients are the sole drivers of segregation. Once
a model for shear-rate-gradient-driven segregation is established, pressure-gradients will
be reintroduced using two more flow configurations – inclined plane flow and planar shear
flow with gravity – in which both segregation mechanisms act simultaneously.
In order to inform continuum model development, we perform two-dimensional discrete element method (DEM) simulations using the open source software LAMMPS [79], which function as “numerical experiments,” and continue to use the grain interaction model described in Chapter 3.2.1. We then coarse-grain DEM simulation results to obtain continuum flow and segregation fields. The coarse-graining technique that we employ stems from the one utilized in Zhang and Kamrin [64] and in Chapter 3 and is described in Appendix B.2. The coupled continuum model that we develop is then validated by comparing its prediction of transient flow and segregation against additional DEM simulations results.

This chapter is organized as follows. In Section 4.2, we discuss the continuum model that we use to describe flow and size-segregation in bidisperse, dense granular materials. Specifically, Section 4.2.1 introduces the mixture theory framework used to describe dense, bidisperse granular mixtures, and in Section 4.2.2, we briefly revisit the local inertial rheology and the nonlocal granular fluidity model for monodisperse granular systems and discuss their extension to bidisperse systems. Then in Section 4.2.3, we hypothesize a model for shear-rate-gradient-driven size-segregation. In Section 4.3 and Section 4.4, we independently determine the two dimensionless material parameters that appear in the shear-strain-rate-driven size-segregation model. Then, in Section 4.5, the proposed segregation model is coupled with the NGF model and applied to both vertical chute flow and annular shear flow to predict the segregation dynamics in transient flow, and the predicted continuum fields are compared against DEM measurements. With a good understanding of the shear-rate-gradient-driven segregation mechanism in hand, in Section 4.6, we turn attention to the pressure-gradient-driven mechanism, introducing an additional pressure-gradient-driven segregation flux term to the continuum model. In Section 4.7, we verify the effectiveness of the model in the inclined plane flow configuration. Finally, in Section 4.8, we validate the full continuum model that accounts for both size-segregation mechanisms in planar shear flow with gravity. In the end, our model demonstrates a level of
fidelity in simultaneously predicting flow and segregation dynamics that has not been previously achieved. We close with a discussion relating our model to others’ work and future steps in Section 4.9.

4.2 Continuum framework

In this section, we discuss the continuum framework used to describe dense, bidisperse granular systems and then propose constitutive models for rheology and size-segregation. Throughout, we utilize a mixture-theory-based approach, which is common in continuum modeling of dense, bidisperse mixtures [e.g., 90 95 97].

4.2.1 Bidisperse systems

We consider two-dimensional granular mixtures consisting of disks with two sizes – large grains with an average diameter of \( d_l \) and small grains with an average diameter of \( d_s \), as shown in Fig. 4.1. In order to rule out the effect of density-based segregation [99], all particles have the same area-density \( \rho_s \). Throughout, we utilize the notational convention, in which we denote large-grain quantities using a superscript \( l \) and small-grain quantities
Grain size | Solid area fraction | Concentration | Velocity | Relative area flux
---|---|---|---|---
Large grains | $d^l$ | $\phi^l$ | $c^l = \phi^l / \phi$ | $v_i^l$ | $w_i^l = c^l(v_i^l - v_i)$
Small grains | $d^s$ | $\phi^s$ | $c^s = \phi^s / \phi$ | $v_i^s$ | $w_i^s = c^s(v_i^s - v_i)$
Mixture | $\bar{d} = c^1d^l + c^sd^s$ | $\phi = \phi^l + \phi^s$ | $1 = c^1 + c^s$ | $v_i = c^1v_i^l + c^sv_i^s$ | $0_i = w_i^l + w_i^s$

Table 4.1: Summary of the quantities introduced to describe dense, bidisperse granular mixtures.

using a superscript $s$, and the important kinematic quantities are summarized in Table 4.1. The species-specific solid area fractions – i.e., the areas occupied by each species per unit total area – are $\phi^l$ and $\phi^s$, respectively, and the total solid area fraction is $\phi = \phi^l + \phi^s$. The concentration of each species then follows as $c^l = \phi^l / \phi$ and $c^s = \phi^s / \phi$, so that $c^l + c^s = 1$. The average mixture grain size is defined as the sizes of both species weighted by their concentrations, $\bar{d} = c^1d^l + c^sd^s$. We make the standard assumption that the total area (or volume for spherical grains) of the dense flows that we study does not change \cite{44, 90, 95, 97}, and therefore $\phi$ remains approximately constant at each point in space and at each point in time during the segregation process. This assumption may be tested by experiments and DEM simulations, in which it is observed that volume dilatation at flow initiation occurs over a much shorter time scale than the process of segregation.

Regarding the kinematics of flow, each species has an associated partial velocity, $v_i^l$ and $v_i^s$, and the mixture velocity is given by $v_i = c^1v_i^l + c^sv_i^s$. The mixture strain rate tensor is then defined using the mixture velocity in the standard way: $\dot{\gamma}_{ij} = (1/2)(\partial v_i / \partial x_j + \partial v_j / \partial x_i)$, where $\dot{\gamma}_{kk} = 0$ since we have assumed that the mixture area (volume) does not change. The equivalent shear strain-rate is defined as $\dot{\gamma} = (2\dot{\gamma}_{ij}\dot{\gamma}_{ij})^{1/2}$. 
Then, the relative area flux for each grain type $\alpha$ is defined as $w_i^\alpha = c^\alpha (v_i^\alpha - v_i)$, so that $w_l^l + w_s^s = 0$. Conservation of mass for each species requires that $Dc^\alpha / Dt + \partial w_i^\alpha / \partial x_i = 0$. Due to the fact that $c^l + c^s = 1$, only one of $c^l$ and $c^s$ is independent. Therefore, we will utilize $c^l$ as the field variable that describes size-segregation in the following. Conservation of mass in terms of large particles is

\[
\frac{Dc^l}{Dt} + \frac{\partial w_l^l}{\partial x_i} = 0. \tag{4.1}
\]

In order to close the system of equations, we require (1) a rheology that relates the strain-rate tensor to the stress and (2) a constitutive equation for the flux $w_i^l$—each of which are discussed in the following subsections.

### 4.2.2 Granular rheology – from monodispersity to bidispersity

In this section, we discuss the rheology of dense, bidisperse granular mixtures. As before, the starting point of this discussion is the local inertial rheology function $\mu_{loc}(I)$. Regarding stress quantities, the mixture Cauchy stress is denoted as $\sigma_{ij} = \sigma_{ji}$, and we define the pressure $P = -(1/3)\sigma_{kk}$, the stress deviator $\sigma'_{ij} = \sigma_{ij} + P\delta_{ij}$, the equivalent shear stress $\tau = (\sigma'_{ij}\sigma'_{ij}/2)^{1/2}$, and the stress ratio $\mu = \tau/P$—all for the mixture. As shown by Rognon et al. [100] and Tripathi and Khakhar [101], the inertial rheology function $\mu_{loc}(I)$ may be straightforwardly generalized from monodisperse to bidisperse systems by defining the inertial number for a bidisperse system as $I = \dot{\gamma}\sqrt{\bar{d}^2\rho_s/P}$, where the average mixture grain size for a bidisperse system $\bar{d}$ has been used in place of $d$ for a monodisperse system.

Then, the same local rheology function $\mu_{loc}(I)$ utilized for the monodisperse system may be used for bidisperse systems without any change to the parameters appearing in the fitting function. This approach neglects the potential effect of new dimensionless quantities that arise in a bidisperse granular system, such as the grain size ratio $d_l/d_s$, but has been shown to capture DEM data well.
To demonstrate this point, consider homogeneous, planar shear of a dense bidisperse system of disks, illustrated in Fig. 4.2(a) for the case of $d^l/d^s = 1.5$ and a system-wide large-grain concentration of $c^l = 0.5$. In this case, no segregation will occur since the flow is homogeneous and no pressure or strain-rate gradients are present. We utilize the DEM procedures described in detail in Chapter 3.2 in order to extract the relationship between $\mu$ and $I$ for bidisperse mixtures with grain size ratios of $d^l/d^s = 1.5, 2.0, 2.5$, and $3.0$ and $c^l = 0.5$. The simulated relationships are plotted in Fig. 4.2(b) using black symbols, along with our monodisperse data from Fig. 3.2(b) plotted as gray symbols. The relationship between $\mu$ and $I$ is observed to be approximately independent of $d^l/d^s$. As for the monodisperse case (Fig. 3.2(b)), the DEM data for bidisperse mixtures of disks may be fit by a Bingham-like functional form:

$$\mu_{\text{loc}}(I) = \mu_s + bI,$$  

(4.2)
where $\mu_s = 0.272$ and $b = 1.168$ are the dimensionless material parameters for monodisperse disks. In this way, we may capture the rheology of bidisperse mixtures in homogeneous planar shear without introducing additional fitting functions or adjustable parameters.

Then, in order to consider inhomogeneous flows, it is necessary to generalize the nonlocal granular fluidity model to the case of dense, bidisperse mixtures. As before, we introduce the granular fluidity $g$ – a positive, scalar field quantity – and recognize that $g$ represents the fluidity of the mixture. Then, we utilize the steady-state form of the NGF model, which relates the stress state, the strain-rate, and the granular fluidity through two constitutive equations: (1) the flow rule

$$\dot{\gamma} = g\mu, \tag{4.3}$$

and (2) the nonlocal rheology

$$g = g_{\text{loc}}(\mu, P) + \xi^2(\mu) \frac{\partial^2 g}{\partial x_i \partial x_i}, \tag{4.4}$$

where $g_{\text{loc}}(\mu, P)$ is the local fluidity function and $\xi(\mu)$ is the stress-dependent cooperativity length. Consistent with the new definition of the inertial number involving $\bar{d}$ and the local inertial rheology function (4.2), the local fluidity function is taken to be

$$g_{\text{loc}}(\mu, P) = \begin{cases} \sqrt{\frac{P}{\rho_s d^2}} \frac{(\mu - \mu_s)}{b\mu} & \text{if } \mu > \mu_s, \\ 0 & \text{if } \mu \leq \mu_s, \end{cases} \tag{4.5}$$

with $\{\mu_s = 0.272, b = 1.168\}$. We utilize an analogous approach to extend the cooperativity length $\xi(\mu)$ to the bidisperse case, in which $d$ for monodisperse grains in (3.5) is replaced by $\bar{d}$ for bidisperse grains:

$$\xi(\mu) = \frac{A\bar{d}}{\sqrt{\mu - \mu_s}}. \tag{4.6}$$
Furthermore, we continue to use the numerical value of the nonlocal amplitude for monodisperse disks, $A = 0.9$, which was determined in Chapter 3. These choices will be tested in later sections by comparing flow fields predicted by the NGF model to measured flow fields in DEM simulations of bidisperse, inhomogeneous flows.

### 4.2.3 Segregation model

We take the flux $w_i$ to be comprised of two contributions – a diffusion flux $w_i^{\text{diff}}$ and a shear-strain-rate-gradient-driven segregation flux $w_i^{\text{seg}}$:

$$ w_i = w_i^{\text{diff}} + w_i^{\text{seg}}. \quad (4.7) $$

Each contribution is discussed further below.

- The diffusion flux acts counter to segregation to mix the species and is taken to be given in the standard form $w_i^{\text{diff}} = -D \left( \partial c^1 / \partial x_i \right)$, where $D$ is the binary diffusion coefficient [102]. From dimensional arguments, we expect

$$ D = C_{\text{diff}} d^2 \dot{\gamma}, \quad (4.8) $$

in which $C_{\text{diff}}$ is a dimensionless material parameter which must be determined [96, 99]. Therefore, we have that the diffusion flux is

$$ w_i^{\text{diff}} = -C_{\text{diff}} d^2 \dot{\gamma} \frac{\partial c^1}{\partial x_i}. \quad (4.9) $$

- Regarding segregation, a major question is what field quantity drives the segregation flux. Gradients of a number of kinematic quantities are possible – e.g., strain-rate, velocity fluctuations, or fluidity. For perspective, we note that recent works [97, 98, 103, 104] have shown that gradients in kinetic stress – which are defined by way of
the velocity fluctuation – correlate well with segregation flux. In the present work, we adopt the simplest approach and hypothesize that the segregation flux is driven by gradients in the shear strain-rate $\dot{\gamma}$ and take the segregation flux to be given in the following phenomenological form:

$$w_{seg}^{i} = C_{seg}^{i} d^{2} c^{1} (1 - c^{1}) \frac{\partial \dot{\gamma}}{\partial x_{i}}. \quad (4.10)$$

The factor $c^{1} (1 - c^{1})$ ensures that segregation ceases when the bidisperse mixture becomes either all large ($c^{1} = 1$) or all small ($c^{1} = 0$) grains, and the factor $d^{2}$ is present for dimensional consistency. The quantity $C_{seg}^{i}$ is a dimensionless material property. While it is possible for $C_{seg}^{i}$ to depend on the size ratio $d^{l}/d^{s}$, we will demonstrate that this effect is negligible in the DEM simulations of Section 4.4 and therefore treat $C_{seg}^{i}$ as a constant, dimensionless material parameter for disks, which will be determined by fitting to DEM simulation results.

Combining (4.9), (4.10), and (4.7) with conservation of mass (4.1), we obtain the following governing equation for $c^{1}$:

$$\frac{D c^{1}}{D t} + \frac{\partial}{\partial x_{i}} \left( -C_{diff} d^{2} \dot{\gamma} \frac{\partial c^{1}}{\partial x_{i}} + C_{seg}^{i} d^{2} c^{1} (1 - c^{1}) \frac{\partial \dot{\gamma}}{\partial x_{i}} \right) = 0, \quad (4.11)$$

where $\{C_{diff}, C_{seg}^{i}\}$ represent two constant dimensionless material parameters that remain to be determined.

### 4.3 Diffusion flux

First, we determine the value of $C_{diff}$ for our dense, bidisperse system of dry, frictional disks. Consider homogeneous planar shear flow of such a bidisperse mixture, as shown in Fig. 4.2(a). Again, no segregation occurs in this setting, since neither of the segregation
Figure 4.3: The binary diffusion coefficient (measured by way of the Mean Square Displacement) versus $\dot{\gamma}d^2$ in homogeneous, steady planar shearing DEM simulations and for grain-size ratios of $d^1/d^s = 1.5, 2.0, 2.5, 3.0, \text{ and } 4.0$. Both axes are normalized by $d^s\sqrt{P_w/\rho_s}$. Each symbol is measured from one DEM simulation of a specified size ratio at one shearing rate. The solid line represents the best fit of a linear relation with $C_{\text{diff}} = 0.20$.

Driving forces – pressure-gradients or shear-strain-rate-gradients – are present \[101\]. During steady, planar shearing, the motion of individual grains in the direction transverse to flow (the $z$-direction in Fig. 4.2(a)) approximates a random walk. Therefore, by measuring the Mean Square Displacement (MSD) of the system of $N$ particles as a function of time, we may determine the binary diffusion coefficient $D$ through \[102, 105-108\]

$$\text{MSD}(t) = \frac{1}{N} \sum_{n=1}^{N} (z_n(t) - z_n(0))^2 = 2Dt. \quad (4.12)$$

We simulate homogeneous, steady planar shear flows for grain-size ratios of $d^1/d^s = 1.5, 2.0, 2.5, 3.0, \text{ and } 4.0$ and at various shearing rates. Indeed, after a sufficiently long time, the measured MSD is linear in time in all cases, allowing us to extract the diffusion coefficient $D$ for each case.

The diffusion coefficient $D$ is plotted against $\dot{\gamma}d^2$ (with both quantities normalized by $d^s\sqrt{P_w/\rho_s}$) in Fig. 4.3. In general, the diffusion coefficient data collapses to a linear relation with $D \sim \dot{\gamma}d^2$ across the range of size ratios considered. A best fit of the slope of the
linear relation – the line in Fig. 4.3 – yields:

\[ C_{\text{diff}} = \frac{D}{\gamma d^2} = 0.20. \]  

(4.13)

In order to further validate the fitted value of \( C_{\text{diff}} \), we have performed a consistency test by considering planar shearing of an initially fully-segregated cell, which is described in Appendix C. In this case, diffusion drives remixing of the two species. Using the fitted value of \( C_{\text{diff}} \) in (4.13), we are able to quantitatively capture the diffusive remixing process, which provides confidence in our fitted value of \( C_{\text{diff}} \).

4.4 Shear-rate-gradient-driven segregation flux

Having independently determined the material parameter \( C_{\text{diff}} \), we next turn to testing the constitutive equation for the shear-rate-gradient-driven segregation flux (4.10) and determining the material parameter \( C_{\text{seg}}^S \) by studying two representative flow configurations – vertical chute flow and annular shear flow.

4.4.1 Vertical chute flow

Consider a dense, bidisperse granular mixture flowing down a long vertical chute with rough parallel walls separated by a distance \( W \) under the action of gravity \( G \), as described in Chapter 3.4.3 for the monodisperse case. Our corresponding DEM set-up for the bidisperse case is shown in Fig. 4.4(a) for \( W = 60\bar{d}_0 \) – where \( \bar{d}_0 \) is the system-wide average grain size. In all cases, we take the chute length to be \( L = 60\bar{d}_0 \) and apply periodic boundary conditions along the \( z \)-direction. The left vertical wall is fixed, and the right wall is fixed in the \( z \)-direction but can move slightly in the \( x \)-direction so as to maintain a constant wall pressure \( P_w \), utilizing the same wall-position control method described in Section 3.2.2.
Figure 4.4: (a) Initial well-mixed configuration for two-dimensional DEM simulation of bidisperse vertical chute flow with 4327 flowing grains. The chute width is $W = 60d_0$. As in Fig. 4.2, black grains on both sides represent rough walls (only large particles are used as wall grains here). (b) Segregated configuration after flowing for a total time of $\tilde{t} = t/ \left( d^2 \sqrt{\rho_s/\rho_w} \right) = 4.3 \times 10^5$. (c) & (d) Spatiotemporal evolution of the large grain concentration $c^l$ and the normalized velocity $(v_{\text{cen}} - v_z) \sqrt{\rho_s/\rho_w}$, respectively. (e) & (f) Spatial profiles of concentration and normalized velocity at three times – $\tilde{t} = 4 \times 10^3, 4 \times 10^4$ and $4 \times 10^5$ – as indicated by the dashed lines in (c) & (d).
Recall that the stress field in vertical chute flow is statically-determinate and given by:

\[
\tau(x) = \phi \rho_s G |x|
\]

\[
P(x) = P_w
\]

\[
\mu(x) = \mu_w |x|/(W/2)
\]

where \( \mu_w = \phi \rho_s G W / (2P_w) \).

We note that while flow is driven by gravity, pressure is constant throughout the chute and no hydrostatic pressure gradients are present. Therefore, segregation occurs only due to shear-strain-rate-gradients, enabling us to consider this effect in isolation.

There are four important dimensionless parameters that describe vertical chute flow of dense bidisperse granular mixtures: (1) \( W/\bar{d}_0 \), the dimensionless chute width; (2) \( \mu_w \), the maximum stress ratio, which occurs at the walls and controls the total flow rate; (3) \( c_0^L(x) \), the initial large-grain concentration, which is not necessarily constant and can be a spatially-varying field; and (4) \( d^L / d^S \), the bidisperse grain-size ratio. Note that the parameters \( \{W/\bar{d}_0, \mu_w, c_0^L, d^L / d^S\} \) are related to the geometry, loads, and initial conditions of the problem and are not material parameters.

As a representative base case, we consider the parameter group \( \{W/\bar{d}_0 = 60, \mu_w = 0.45, c_0^L = 0.5, d^L / d^S = 1.5\} \). We then run the corresponding DEM simulation starting from the well-mixed initial configuration shown in Fig. 4.4(a) and observe that after a simulation time of \( \tilde{t} = t / (d^S \sqrt{\rho_s / P_w}) = 4.3 \times 10^5 \) the large, dark grains segregate towards the regions near the walls where the shear-strain-rate is greatest, while the small, light (in color) grains gather in bands just inside these regions, as shown in Fig. 4.4(b). A well-mixed core persists along the center of the vertical chute where the shear strain-rate is nearly zero. To obtain a more quantitative picture of the segregation process, we coarse-grain the concentration field \( c^L \) and the velocity field \( v_z \) in both space and time and plot contours of the spatiotemporal evolution of \( c^L \) and \( v_z \) in Figs. 4.4(c) and (d), respectively. Both the concentration and velocity fields evolve quickly in time during flow initiation. Then, over longer times, the
Figure 4.5: Collapse of $C_{\text{diff}}d^3\gamma(\partial c^1/\partial x) / (\partial c^1 / \partial x)$ versus $d^3 c^1 (1 - c^1)(\partial \gamma / \partial x)$ for several cases of vertical chute flow of bidisperse disks. Symbols represent coarse-grained quasi-steady DEM field data, and the solid line is the best linear fit using $C_{\text{seg}} = 0.23$.

evolution of these fields becomes slower and may eventually be regarded as quasi-steady. For the example shown in Fig. 4.4, a true steady-state, corresponding to a fully-segregated configuration, is not reached within the simulated time window. Spatial profiles of the concentration and velocity fields at three snapshots in time – $\tilde{t} = t / (d^3\sqrt{\rho_s/P_w}) = 4 \times 10^3, 4 \times 10^4$ and $4 \times 10^5$ as indicated by the dashed lines in Figs. 4.4(c) and (d) – are plotted in Figs. 4.4(e) and (f). These three snapshots correspond to early, medium, and late times with respect to the segregation process. The spatial $c^1$ profiles shown in Fig. 4.4(e) demonstrate the transition from a well-mixed state to a segregated state with large-grain-rich and small-grain-rich regions. The normalized velocity fields $(v_{\text{cen}} - v_z)\sqrt{\rho_s/P_w}$ – relative to the velocity at the center of the chute, $v_{\text{cen}} = v_z(x = 0)$ – show that the velocity field rapidly develops into a steady flow field (Fig. 4.4(f)) – even while the segregation process is still occurring, and the $c^1$ field continues to evolve.

At long times, near the end of the simulated time window ($\tilde{t} = t / (d^3\sqrt{\rho_s/P_w}) \gtrsim 3 \times 10^5$), the concentration field evolves very slowly – $Dc^1 / Dt \approx 0$ – and therefore, according to equations (4.1) and (4.7), the total flux is approximately zero – $w_i = w_{\text{diff}}^i + w_{\text{seg}}^i \approx 0_i$ – meaning that the segregation flux is approximately balanced by the diffusion flux in this quasi-steady flow regime. Then, using the expressions for the two fluxes, equations (4.9)
and (4.10), this observation implies that

\[ C_{\text{diff}} d^2 \gamma \frac{\partial c^l}{\partial x} \approx C_{\text{seg}}^S d^2 (1 - c^l) \frac{\partial \gamma}{\partial x}. \]  

(4.15)

The field quantities appearing in this expression may be obtained by coarse-graining the DEM data in the quasi-steady regime. Therefore, since \( C_{\text{diff}} \) has been previously determined, (4.15) may be used to determine the parameter \( C_{\text{seg}}^S \) as follows. First, we acquire the field quantities \( c^l \) (and hence \( \bar{d} \)) and \( v_z \) by spatially coarse-graining 152 evenly-distributed snapshots in time in the quasi-steady regime \( (\tilde{t} > 3 \times 10^5) \)\(^1\). Then, we average these fields in time, yielding fields that only depend on the spatial coordinate \( x \), and take spatial gradients to obtain \( \partial c^l / \partial x, \gamma = \partial v_z / \partial x \), and \( \partial \gamma / \partial x = \partial^2 v_z / \partial x^2 \)\(^2\). Next, as suggested by (4.15), we plot \( C_{\text{diff}} d^2 \gamma (\partial c^l / \partial x) \) versus \( d^2 (1 - c^l) (\partial \gamma / \partial x) \) in Fig. 4.5, in which each point represents a unique \( x \)-position. A linear relation is observed, supporting our choice for the form of the constitutive equation for the segregation flux (4.10). In order to obtain further evidence for this choice, we consider four additional cases: (1) a lower flow rate \( \{W/\bar{d}_0 = 60, \mu_w = 0.375, c_0^l = 0.5, d^l/d^s = 1.5\} \); (2) a narrower channel \( \{W/\bar{d}_0 = 40, \mu_w = 0.45, c_0^l = 0.5, d^l/d^s = 1.5\} \); (3) more large grains \( \{W/\bar{d}_0 = 60, \mu_w = 0.45, c_0^l = 0.75, d^l/d^s = 1.5\} \); and (4) a larger size ratio \( \{W/\bar{d}_0 = 60, \mu_w = 0.45, c_0^l = 0.5, d^l/d^s = 3.0\} \). Coarse-graining the quasi-steady fields for each case and including the field data in Fig. 4.5, we observe a strong linear collapse. Finally, the dimensionless material parameter \( C_{\text{seg}}^S \) may be obtained from the slope of the linear relation in Fig. 4.5 (indicated by the solid line). We determine the numerical value for disks to be \( C_{\text{seg}}^S = 0.23 \) and note that this value indeed appears to be independent of the grain-size ratio \( d^l/d^s \).

\(^{1}\)Results are not particularly sensitive to the quasi-steady regime criterion, and we only provide this value as a guideline.

\(^{2}\)A detailed description of our coarse-graining technique may be found in Appendix \( \text{B.2} \)
4.4.2 Annular shear flow

The constitutive equation for the segregation flux \((\text{4.10})\) and the fitted value of the material parameter for disks \(C_{\text{seg}}^S = 0.23\) should be general across different flow configurations. To test this, we apply the same process described in the preceding section for vertical chute flow to a different flow configuration – annular shear flow. In this configuration, flow is boundary-driven, but like the vertical chute, it is a constant-pressure configuration that eliminates hydrostatic pressure gradients and displays only shear-rate-gradient-driven size-segregation.

Our DEM simulations of annular shear flow of a dense, bidisperse granular mixture follow the procedure described in Chapter 3.4.2 for the monodisperse case. Consider a dense, bidisperse granular mixture in a two-dimensional annular shear cell with rough circular walls of inner radius \(R\) and outer radius \(R_o\), shown in Fig. 4.6(a). The circumferential velocity of the inner wall is prescribed to be \(v_w\), and its radial position is fixed. The outer wall does not rotate, and its radial position fluctuates slightly so as to maintain a constant imposed wall pressure \(P_w\), utilizing a wall-position control method analogous to that described in Section 3.2.2. In this configuration, flow tends to localize near the inner wall, with the velocity field rapidly decaying with radial position. We choose the outer radius \(R_o\) to be sufficiently large so that it does not affect the resulting flow and segregation fields, and based on our experience, we take \(R_o = 2R\). Therefore, the role of the outer wall is simply to apply a far-field pressure, and otherwise, it does not affect the flow and segregation fields. Also, as in Chapter 3.4.2, we simulate the full shear cell instead of applying periodic boundary conditions on a slice [27, 41, 78].
Figure 4.6: (a) Initial well-mixed configuration for two-dimensional DEM simulation of bidisperse annular shear flow with 40108 flowing grains. The inner wall radius is \( R = 60d_0 \), and the outer wall radius is \( R_o = 2R \). The circular walls consist of rings of large particles. (b) Segregated configuration after flowing for a total time of \( \tilde{t} = t / (R/v_w) = 584 \). (c) & (d) Spatiotemporal evolution of the large grain concentration \( c_l \) and the normalized rotational velocity \( v_\theta/v_w \) respectively. (e) & (f) Spatial profiles of concentration and normalized velocity at three times \( \tilde{t} = 5, 50 \) and 500 – as indicated by the dashed lines in (c) & (d).
Recall that the stress field in annular shear flow is statically-determinate and given by:

\[ \tau(r) = \tau_w(R/r)^2 \]
\[ P(r) = P_w \]
\[ \mu(r) = \mu_w(R/r)^2 \]

with \( \mu_w = \tau_w/P_w \),

where \( \tau_w \) is the inner-wall shear stress. It is important to note that \( \tau_w \) is not directly prescribed in our DEM simulations. Instead, the inner-wall velocity \( v_w \) is prescribed, and \( \tau_w \) and hence \( \mu_w \) arise as a result, as illustrated in Fig. 3.4(b) for the monodisperse case. Therefore, the four important dimensionless parameters that describe annular shear flow of dense bidisperse granular mixtures are (1) \( R/d_0 \), the dimensionless inner-wall radius; (2) \( \bar{v}_w = (v_w/R)\sqrt{\pi \rho_s d_0^2/(4P_w)} \), the dimensionless inner-wall velocity, which determines \( \tau_w \) and \( \mu_w \); (3) \( c_{l0}(r) \), the initial large-grain concentration; and (4) \( d_l/d_s \), the bidisperse grain-size ratio.

We choose a representative base case of quasi-static annular shear flow identified by the parameter set \( \{R/d_0 = 60, \bar{v}_w = 0.01, c_{l0} = 0.5, d_l/d_s = 1.5\} \). The well-mixed initial configuration for the base-case DEM simulation is shown in Fig. 4.6(a), and the segregated configuration after driving flow for a total time of \( \bar{t} = t/(R/v_w) = 584 \) is shown in Fig. 4.6(b). The large, dark grains segregate into a ring near the inner wall, while the small, light grains form a band just outside this region. Outside of these bands, where the shear strain-rate is very small, the grains remain well-mixed. Contours of the coarse-grained concentration field \( c^l \) and the tangential velocity field \( v_{\theta}/v_w \) are shown in Figs. 4.6(c) and (d), illustrating the time-evolution of these fields. Snapshots of the spatial profiles of the concentration and velocity fields at selected stages of the segregation dynamics – \( \bar{t} = t/(R/v_w) = 5, 50, \) and 500 as indicated by the dashed lines in Figs. 4.6(c) and (d) – are shown in Figs. 4.6(e) and (f). The radial \( c^l \) profiles demonstrate the formation of large-grain-rich and small-grain-rich regions with a persistent well-mixed far-field. As in the case of vertical chute flow,
Figure 4.7: Collapse of $C_{\text{diff}} \gamma (\partial c^1 / \partial r)$ versus $d^2 c^1 (1 - c^1) (\partial \dot{\gamma} / \partial r)$ for several cases of annular shear flow of bidisperse disks. Symbols represent coarse-grained, quasi-steady DEM field data, and the solid line is the best linear fit using $C_{\text{seg}}^S = 0.23$.

The velocity field quickly develops into a quasi-steady flow field – while the large grain concentration field $c^1$ evolves over a longer time-scale before approaching a quasi-steady state near the end of our simulated time window. The flowing zone is localized near the inner wall with slow creeping flow observed far from the wall.

Again, at long times, near the end of the simulated time window ($\tilde{t} = t / (R/v_w) \gtrsim 500$), the concentration field evolves very slowly, which we identify as the quasi-steady regime. In this regime, the segregation and diffusion fluxes approximately balance, implying that

$$C_{\text{diff}} d^2 \gamma \frac{\partial c^1}{\partial r} \approx C_{\text{seg}}^S d^2 c^1 (1 - c^1) \frac{\partial \dot{\gamma}}{\partial r}. \quad (4.17)$$

As for the case of vertical chute flow, we spatially coarse-grain the DEM data for 144 evenly-distributed snapshots in time in the quasi-steady regime ($\tilde{t} \gtrsim 500$) to obtain field quantities in (4.17) and then time-average these fields (before taking spatial derivatives). Next, we plot $C_{\text{diff}} d^2 \gamma (\partial c^1 / \partial r)$ versus $d^2 c^1 (1 - c^1) (\partial \dot{\gamma} / \partial r)$ in Fig. 4.7 with each point representing a unique $r$-position. Finally, this process is repeated for four additional cases: (1) a lower inner-wall velocity $\{R/d_0 = 60, v_w = 0.001, c^1_0 = 0.5, d^1/d^s = 1.5\}$; (2) a smaller inner-wall radius $\{R/d_0 = 40, v_w = 0.01, c^1_0 = 0.5, d^1/d^s = 1.5\}$; (3) more large grains...
\( \{ R/d_0 = 60, v_w = 0.01, \epsilon^l_0 = 0.75, d^l/d^s = 1.5 \} \); and (4) a larger size ratio \( \{ R/d_0 = 60, v_w = 0.01, \epsilon^l_0 = 0.5, d^l/d^s = 3.0 \} \), and the coarse-grained, quasi-steady fields are included in the data plotted in Fig. 4.7. Collectively, we observe a strong collapse to a linear relation. Crucially, the slope of the linear relation in Fig. 4.7 (indicated by the solid line) gives the same value for the dimensionless material parameter obtained by fitting to vertical chute flow data, \( C_{seg}^S = 0.23 \). This observation of agreement in the best fit value of \( C_{seg}^S \) obtained via two independent routes provides support for our choice of the constitutive equation for the segregation flux (4.10) and the fitted value of \( C_{seg}^S \) for disks.

### 4.5 Validation of shear-strain-rate-gradient-driven segregation flux in transient flow

With a calibrated model for shear-strain-rate-gradient-driven size-segregation in hand (4.11), we may now couple (4.11) with the NGF model, (4.3) and (4.4), in order to obtain predictions of the simultaneous, transient evolution of segregation and flow fields, using a fixed set of material parameters for disks:

\[
\{ \mu_s = 0.272, b = 1.168, A = 0.9, C_{diff} = 0.20, C_{seg}^S = 0.23 \}. \tag{4.18}
\]

In the preceding section, we only used DEM data from the quasi-steady regime to inform the model and determine the parameter \( C_{seg}^S \). In this section, we compare model predictions of the transient evolution of segregation and flow fields to the DEM data for both vertical chute flow and annular shear flow without further parameter adjustment as a validation test of the model.
4.5.1 Vertical chute flow

Continuum model predictions are obtained by solving the governing partial differential equations using finite-differences. Summarizing the coupled boundary/initial-value problem for flow and segregation in the context of vertical chute flow, the unknown fields are the strain-rate $\dot{\gamma} = \partial v_z / \partial x$, the granular fluidity $g$, and the large-grain concentration $c^l$. The governing field equations are (1) the flow rule,

$$\dot{\gamma} = g\mu, \quad (4.19)$$

(2) the nonlocal rheology,

$$g = g_{\text{loc}}(\mu(x), P_w) + \xi^2 (\mu(x)) \frac{\partial^2 g}{\partial x^2} \quad (4.20)$$

with $g_{\text{loc}}$ and $\xi$ given through (4.5) and (4.6), respectively, and (3) conservation of mass for the large grains,

$$\frac{\partial c^l}{\partial t} + \frac{\partial}{\partial x} \left( -C_{\text{diff}} d^l \gamma \frac{\partial c^l}{\partial x} + C_{\text{seg}} S d^2 c^l (1 - c^l) \frac{\partial \dot{\gamma}}{\partial x} \right) = 0, \quad (4.21)$$

where $d = c^l d^l + (1 - c^l) d^s$. Since the problem is statically-determinate, the stress ratio field $\mu(x)$ is given through (4.16), and the balance of momentum does not enter the governing equations.

Regarding boundary conditions, we impose Dirichlet fluidity boundary conditions at the walls - i.e., $g = g_{\text{loc}}(\mu_w, P_w)$ at $x = 0$ and $x = W$ - as well as no flux boundary conditions at the walls - i.e., $w^l = -C_{\text{diff}} d^l \gamma (\partial c^l / \partial x) + C_{\text{seg}} S d^2 c^l (1 - c^l) (\partial \dot{\gamma} / \partial x) = 0$ at $x = 0$ and $x = W$. Due to the time derivative in (4.21), an initial condition for the concentration field $c^l_0(x) = c^l(x,t = 0)$ is required. In order to account for the concentration fluctuations inherent in the initial state, we obtain the coarse-grained $c^l$-field from the initial DEM configuration for each case and utilize this field as the initial condition field $c^l_0(x)$ in the
respective continuum simulation.

Then, for a given case identified through a set of input parameters \{W/\tilde{d}O, \mu_w, c^l_0(x), \tilde{d}^l/d^s\}, we obtain numerical predictions of the coupled model utilizing finite differences as follows. First, at a given point in time, the concentration field \(c^l(x)\) is known, allowing the average grain-size field to be calculated through \(\bar{d} = c^l d^l + (1 - c^l) d^s\). Using the stress ratio field \(\mu(x)\) for vertical chute flow (4.14), the local fluidity \(g_{loc}(\mu, P)\) and the cooperativity length \(\xi(\mu)\) – equations (4.5) and (4.6) – may be calculated at each spatial grid point. Then, the nonlocal rheology (4.20) may be used to solve for the fluidity field \(g(x)\) at the current step, using central differences in space. The strain-rate field follows using (4.19), which may be integrated to obtain the velocity field \(v_z(x)\). Next, (4.21) is used to determine the concentration field at the next time step utilizing the forward Euler method and central differences in space with one modification – the gradient of \(c^l\) appearing in the diffusion flux term in (4.21) is treated implicitly in order to improve numerical stability. This completes one time step, and this process is repeated to step forward in time and calculate the transient evolution of the concentration and flow fields – \(c^l(x, t)\) and \(v_z(x, t)\). In our finite-difference calculations, we utilize a fine spatial resolution of \(\Delta x \ll \bar{d}\), and we have verified that the time-step is sufficiently small in order to ensure stable, accurate results.

We compare predictions of the coupled, continuum model to DEM data for all five cases of vertical chute flow considered in Section 4.4.1 – (1) base case, (2) lower flow rate, (3) narrower chute width, (4) more large grains, and (5) larger grain-size ratio – in order to test the generality of the model. Figure 4.8 summarizes the comparisons for these five cases. The first column of Fig. 4.8 shows the spatiotemporal contours of the evolution of \(c^l\) measured in the DEM simulations for each case, and the second column shows comparisons of the DEM simulations (solid lines) and the continuum predictions (dashed lines) for the \(c^l\) field at four time snapshots – \(\tilde{t} = t/ \left( d^s \sqrt{\rho_s/P_w} \right) = 4 \times 10^3, 2 \times 10^4, 1 \times 10^5\) and \(4 \times 10^5\) – indicated by the horizontal dashed lines in the first column of Fig. 4.8. Based on Fig. 4.8, the coupled model generally does a good job capturing the salient features of the evolution
of the $c^1$ field across all cases. For instance, for the narrower chute case shown in Fig. 4.8(c), the segregation process nearly completes within the simulated time window with the mixed core along the center of the chute nearly disappearing, and the continuum model prediction captures this observation well.

Regarding flow fields, comparisons of the DEM-simulated and continuum-model-predicted quasi-steady, normalized velocity fields at $\tilde{t} = 4 \times 10^5$ are shown in the third column of Fig. 4.8. Since the velocity field evolves minimally during the segregation process, only the flow field at long time is shown. We note that the velocity field is very well-predicted in all cases – including the creeping regions far from the wall. This favorable comparison
Figure 4.8: Continued: (d) More large grains case \( \{ W/\bar{d}_0 = 60, \mu_w = 0.45, c_0^1 = 0.75, d_l/d_s = 1.5 \} \); (e) Larger size ratio case \( \{ W/\bar{d}_0 = 60, \mu_w = 0.45, c_0^1 = 0.5, d_l/d_s = 3.0 \} \). For each case, the first column shows spatiotemporal contours of the evolution of \( c^1 \) measured in the DEM simulations. The second column shows comparisons of the DEM simulations (solid lines) and continuum model predictions (dashed lines) of the \( c^1 \) field at four time snapshots representing different stages of segregation: \( \tilde{t} = 4 \times 10^3, 2 \times 10^4, 1 \times 10^5 \) and \( 4 \times 10^5 \) in the sequence of top left, top right, bottom left, bottom right. The third column shows comparisons of the simulated and predicted quasi-steady, normalized velocity profiles at \( \tilde{t} = 4 \times 10^5 \).

provides support of our generalization of the NGF model to bidisperse granular systems discussed in Section 4.2.2 – in particular, the choices to use the average grain size \( \bar{d} \) in the expression for the cooperativity length (4.6) and to continue to use the numerical value for the nonlocal amplitude determined for monodisperse systems, \( A = 0.9 \), without refitting. Overall, the coupled continuum model is capable of quantitatively predicting both the flow fields and the segregation dynamics in vertical chute flow.

### 4.5.2 Annular shear flow

We utilize an analogous approach to obtain continuum model predictions for the transient evolution of concentration and flow fields in annular shear flow. The stress field in annular shear is given by (4.16), and the governing equations (4.19), (4.20), and (4.21) are modified
our continuum simulations, we iteratively adjust the value of \( \mu \) in our DEM simulations in order to achieve the target value of \( v_w \). Slightly to account for the divergence operator in cylindrical coordinates. Also, since \( v_w \), not \( \mu_w \), is specified in our DEM simulations of annular shear, while \( \mu_w \) is specified in our continuum simulations, we iteratively adjust the value of \( \mu_w \) input into our continuum simulations in order to achieve the target value of \( v_w \) in the predicted quasi-steady flow field. Otherwise, our approach is the same. Dirichlet fluidity boundary conditions and no flux boundary conditions are imposed at the walls, and the initial concentration field is extracted from the initial DEM configuration for each case.

Then, we validate continuum model predictions against DEM data in the five cases...
of annular shear flow discussed in Section 4.4.2 – (1) base case, (2) lower inner-wall velocity, (3) smaller inner-wall radius, (4) more large grains, and (5) larger grain-size ratio. Figure 4.9 summarizes the comparisons for these five cases and is organized in the same manner as Fig. 4.8. Again, the coupled, continuum model does a good job capturing the segregation dynamics and the quasi-steady flow field and the changes in these fields induced by changing the input parameters.
4.6 Addition to the segregation model – Pressure-gradient-driven segregation flux

To this point, we have solely considered shear-strain-rate-driven size-segregation, focusing on two flow configurations that isolate this mechanism. Now that a predictive continuum model for this mechanism has been established, we return to pressure-gradient-driven size-segregation in order to incorporate this mechanism and obtain a more general model. As in the preceding section, our approach is to first propose a constitutive equation for the pressure-gradient-driven segregation flux based on previous works in the literature and dimensional arguments. This constitutive equation will then be added to the segregation model and tested against DEM simulations of flow in two new configurations – inclined plane flow and planar shear flow with gravity – in which both shear-strain-rate-gradient-driven and pressure-gradient-driven size-segregation are present.

Following Hill and Tan [103], we posit that the segregation flux may be additively decomposed into a term associated with shear-strain-rate-gradient driven segregation, \( w^S_i \), given through (4.10), and a term associated with pressure-gradient-driven segregation, \( w^P_i \), so that \( w^\text{seg}_i = w^S_i + w^P_i \). Then, we expect that \( w^P_i \) acts along negative pressure gradients, so that large grains will tend to rise to the top of a flowing granular media experiencing hydrostatic pressure gradients. Additionally, the prefactor of \( w^P_i \) should involve the factor \( c^1(1-c^1) \) in order to ensure that segregation ceases when the mixture becomes either all large or all small grains as well as a factor \( \dot{\gamma} \), so that segregation ceases when there is no flow. Therefore, our expected scaling for the pressure-gradient-driven segregation flux is

\[
  w^P_i \propto -\dot{\gamma}c^1(1-c^1) \frac{\partial P}{\partial x_i}.
\]

The remaining prefactor must have units of [\( \text{Length}^3/\text{Force} \)], which using \( \bar{d} \) as the characteristic length-scale and \( P\bar{d} \) as the characteristic force-scale, we take to be \( \bar{d}^2/P \). Therefore,
we propose the following constitutive equation for the pressure-gradient-driven segregation flux:

\[ w_P^i = -C_{\text{seg}}^P \frac{d^2 \gamma}{d \bar{\gamma}} c^l (1 - c^l) \frac{\partial P}{\partial x_i}, \quad (4.22) \]

where \( C_{\text{seg}}^P \) is an additional dimensionless material parameter which scales the rate of pressure-gradient-driven segregation. We emphasize that the hypothesized constitutive equation (4.22) is based on a set of minimal requirements, and it is possible – if not likely – that the flux will depend on other dimensionless quantities, such as the inertial number \( I \) or the grain-size ratio \( d^l/d^s \). Indeed, we will show that \( d^l/d^s \) does have an additional effect on the pressure-gradient-driven segregation flux that was not present in the shear-rate-gradient-driven segregation flux. In the following sections, we will use a similar approach to determine the dimensionless material parameter \( C_{\text{seg}}^P \) and test the constitutive equation (4.22) as was utilized in Sections 4.4 and 4.5.

Adding the constitutive equation (4.22) to the segregation model in Section 4.2.3, the total segregation flux now accounts for both mechanisms:

\[ w_{\text{seg}}^i = -C_{\text{seg}}^P \frac{d^2 \gamma}{d \bar{\gamma}} c^l (1 - c^l) \frac{\partial P}{\partial x_i} + C_{\text{seg}}^S d^2 c^l (1 - c^l) \frac{\partial \dot{\gamma}}{\partial x_i}, \quad (4.23) \]

and using (4.23) in conservation of mass (4.1), we obtain the following governing equation for \( c^l \):

\[ \frac{Dc^l}{Dt} + \frac{\partial}{\partial x_i} \left[ -C_{\text{seg}}^P \frac{d^2 \gamma}{d \bar{\gamma}} c^l (1 - c^l) \frac{\partial P}{\partial x_i} + C_{\text{seg}}^S d^2 c^l (1 - c^l) \frac{\partial \dot{\gamma}}{\partial x_i} - C_{\text{diff}} d^2 \dot{\gamma} \frac{\partial c^l}{\partial x_i} \right] = 0, \quad (4.24) \]

with the dimensionless material parameter set \{ \( C_{\text{diff}} = 0.20, C_{\text{seg}}^S = 0.23, C_{\text{seg}}^P \) \}.

### 4.7 Inclined plane flow

Inclined plane flow is a broadly studied flow configuration [7, 11, 30, 58], which we will utilize to determine the value of the material parameter \( C_{\text{seg}}^P \) and test the coupled model.
Figure 4.10: (a) Initial well-mixed configuration for two-dimensional DEM simulation of bidisperse inclined plane flow with 4311 flowing grains. The layer thickness is $H = 60\bar{d}_0$ with $\bar{d}_0$ the global mean particle size, and the inclination angle is $\theta = 20^\circ$. Black grains represent the bottom, fixed surface. (b) Segregated configuration after flowing for a total time of $\tilde{t} = t/\sqrt{d^3/G} = 2.45 \times 10^4$. (c) & (d) Spatiotemporal evolution of the large grain concentration $c_1$ and the normalized velocity down the incline, $v_x/\sqrt{G\bar{d}}$, respectively. (e) & (f) Spatial profiles of concentration and normalized velocity at three times – $\tilde{t} = 2 \times 10^2$, $2 \times 10^3$, and $2 \times 10^4$ – as indicated by the dashed lines in (c) & (d).
in the presence of hydrostatic pressure gradients. Consider a dense, bidisperse granular mixture flowing down a long inclined surface under the action of gravity $G$ with a surface inclination angle $\theta$ and a layer thickness $H$. Figure 4.10(a) shows a representative DEM setup for a layer thickness of $H = 60\bar{d}_0$ and an inclination angle of $\theta = 20^\circ$. The base of the inclined plane ($z = H$) consists of a layer of fixed large grains, and the top of the layer ($z = 0$) is a free surface. Periodic boundary conditions are employed along the direction of the inclined plane – i.e., the $x$-direction. Throughout, we take the length along the periodic direction to be $60\bar{d}_0$.

The stress distribution in the layer is statically-determinate and given by:

$$
\tau(z) = \phi \rho_s G z \sin \theta \\
P(z) = \phi \rho_s G z \cos \theta \\
\mu(z) = \tan \theta.
$$

(4.25)

Note that the stress ratio $\mu = \tan \theta$ is spatially constant in this flow configuration and given through the inclination angle $\theta$. The four important dimensionless parameters that describe inclined plane flow of dense bidisperse granular mixtures are (1) $H/\bar{d}_0$, the dimensionless layer thickness, (2) $\theta$, the inclination angle, which controls the total flow rate, (3) $c^l_0(z)$, the initial large-grain concentration field, and (4) $d^l/d^s$, the bidisperse grain-size ratio.

We choose a representative base case of inclined plane flow associated with the parameter set \{\(H/\bar{d}_0 = 60, \theta = 20^\circ, c^l_0 = 0.5, d^l/d^s = 1.5\)\}. The well-mixed initial configuration corresponding to the base-case DEM simulation is shown in Fig. 4.10(a). As flow and segregation progress, small grains move towards the bottom of the layer, while large grains segregate towards the top free surface. The segregated configuration after a total time of $\tilde{t} = t/\sqrt{d^s/G} = 2.45 \times 10^4$ is shown Fig. 4.10(b). Contours of the coarse-grained large-grain concentration and the normalized velocity field down the incline $v_x/\sqrt{Gd^s}$ are shown in Figs. 4.10(c) and (d), demonstrating the dynamics of the segregation and flow fields. Snapshots of the spatial profiles of the concentration and velocity fields at three
selected points in time – \( \tilde{t} = 2 \times 10^2, 2 \times 10^3, \) and \( 2 \times 10^4 \) as indicated by the dashed lines in Figs. 4.10(c) and (d) – are plotted in Figs. 4.10(e) and (f). The concave shape of the flow field \( v_x(z) \) is consistent with the so-called “Bagnold profile” for flow down an inclined plane \( [7, 30] \) – \( v_x(z) \propto H^{3/2} - z^{3/2} \) – which is obtained by integrating the strain-rate field predicted by the local inertial rheology over the thickness of the layer. A quasi-steady state in both the concentration and flow fields is attained at sufficiently long times.

Both hydrostatic pressure-gradients and shear-strain-rate-gradients are present in inclined plane flow. It is notable that due to the shape of the velocity profile (Fig. 4.10(f)), the shear-strain-rate is greatest at the bottom of the layer. Therefore, shear-rate-gradients drive smaller grains towards the surface (lower shear-rate region), while pressure-gradients drive smaller grains to the bottom of the layer (higher pressure region) – i.e., shear-rate-gradient-driven and pressure-gradient-driven segregation fluxes are opposed. The observation that small grains segregate towards the bottom of the layer (Figs. 4.10(b) and (c)) suggests that pressure-gradient-driven segregation dominates shear-rate-gradient-driven segregation in this configuration. This feature makes inclined plane flow a good configuration for determining the numerical value of the material parameter \( C_{\text{seg}}^p \).

For the base case, a quasi-steady state for both the concentration and flow fields is reached after \( \tilde{t} \gtrsim 1.5 \times 10^4 \). In this regime, \( Dc^1 / Dt \approx 0 \), and the diffusion flux approximately balances the total segregation flux, \( w^\text{diff}_i + w^S_i + w^P_i \approx 0_i \), which implies that

\[
C_{\text{seg}}^S d^2 c^1 (1 - c^1) \frac{\partial \dot{\gamma}}{\partial z} - C_{\text{diff}} d^2 \dot{\gamma} \frac{\partial c^1}{\partial z} \approx C_{\text{seg}}^P \frac{d^2 \dot{\gamma}}{P} c^1 (1 - c^1) \frac{\partial P}{\partial z}.
\]

We spatially coarse-grain the DEM data for 139 evenly-distributed snapshots in time in the quasi-steady regime (\( \tilde{t} \gtrsim 1.5 \times 10^4 \)) to obtain the field quantities in (4.26) – i.e., \( c^1, \tilde{d}, \) and \( v_x \) in addition to \( P \) and \( \partial P / \partial z \) which are known and therefore not determined by coarse-graining – and then time-average these fields, before taking spatial derivatives to acquire \( \partial c^1 / \partial z, \dot{\gamma} = \partial v_x / \partial z, \) and \( \partial \dot{\gamma} / \partial z \). Additionally, the values of \( C_{\text{diff}} \) and \( C_{\text{seg}}^S \)
Figure 4.11: Collapse of $C_{\text{seg}}^S d^2 c^1 (1 - c^1) (\partial \gamma / \partial z) - C_{\text{diff}}^S d^2 \gamma (\partial c^1 / \partial z)$ versus $(d^2 \gamma / P) c^1 (1 - c^1) (\partial P / \partial z)$ for several cases of inclined plane flow of bidisperse disks with a grain-size ratio of $d^l / d^s = 1.5$. Symbols represent coarse-grained, quasi-steady DEM field data, and the solid line is the best linear fit using $C_{\text{seg}}^P = 0.35$.

are known and not further adjusted. Next, as suggested by (4.26), we plot $C_{\text{seg}}^S d^2 c^1 (1 - c^1) (\partial \gamma / \partial z) - C_{\text{diff}}^S d^2 \gamma (\partial c^1 / \partial z)$ versus $(d^2 \gamma / P) c^1 (1 - c^1) (\partial P / \partial z)$ in Fig. 4.11 in which each point represents a unique $z$-position. This process is repeated for three additional cases: (1) a lower inclination angle $\{H / d_0 = 60, \theta = 18^\circ, c^1_0 = 0.5, d^l / d^s = 1.5\}$; (2) a thinner layer $\{H / d_0 = 40, \theta = 20^\circ, c^1_0 = 0.5, d^l / d^s = 1.5\}$; and (3) more large grains $\{H / d_0 = 60, \theta = 20^\circ, c^1_0 = 0.75, d^l / d^s = 1.5\}$, and the coarse-grained, quasi-steady fields are included in the data plotted in Fig. 4.11. The collapse is comparatively noisier than that observed in the case of shear-rate-gradient-driven segregation; however, a dependence is evident, which may be fit by a linear relation. Then, the dimensionless material parameter $C_{\text{seg}}^P$ is obtained from the slope of the best-fit linear relation in Fig. 4.11 (indicated by the solid line) and is determined to be $C_{\text{seg}}^P = 0.35$ for a grain-size ratio of $d^l / d^s = 1.5$. We note that we observe the numerical value of $C_{\text{seg}}^P$ to depend upon the grain-size ratio. For example, for a case with a larger size ratio $\{H / d_0 = 60, \theta = 20^\circ, c^1_0 = 0.5, d^l / d^s = 3.0\}$, we find that $C_{\text{seg}}^P = 0.65$. Therefore, this data is not included in Fig. 4.11. More completely characterizing the dependence of the pressure-gradient-driven segregation flux on the grain-size ratio will be the subject of future work.
Figure 4.12: Comparisons of the coupled continuum model predictions with corresponding DEM simulation results during transient flow and for five inclined plane flow test cases: (a) Base case \{H/d_0 = 60, \theta = 20^\circ, c_0^1 = 0.5, d^1/d^s = 1.5\}; (b) Lower flow-rate case \{H/d_0 = 60, \theta = 18^\circ, c_0^1 = 0.5, d^1/d^s = 1.5\}; (c) Smaller layer thickness case \{H/d_0 = 40, \theta = 20^\circ, c_0^1 = 0.5, d^1/d^s = 1.5\}. Continued on the next page.

The calibrated model for both shear-rate-gradient-driven and pressure-gradient-driven size-segregation (4.24) may now be coupled with the NGF model, (4.3) and (4.4), and used to obtain predictions of the transient evolution of segregation and flow fields. We use a fixed set of material parameters for disks with a size-ratio of $d^1/d^s = 1.5$, \{\mu_s = 0.272, b = 1.168, A = 0.9, C_{\text{diff}} = 0.20, C_{\text{seg}}^S = 0.23, C_{\text{seg}}^P = 0.35\}. Continuum model predictions are numerically obtained as described in Section 4.5.1 for vertical chute flow. We utilize a Dirichlet fluidity boundary condition at the rough bottom – i.e., $g = g_{\text{loc}}(\mu = \tan \theta, P = \phi \rho_s GH)$ at $z = H$ – and a homogeneous Neumann fluidity boundary condition at the free surface – $\partial g/\partial z = 0$ at $z = 0$ – in addition to no flux boundary conditions at both the bottom
Figure 4.12: Continued: (d) More large grains case \( \{ H/d_0 = 60, \theta = 20^\circ, c^1_0 = 0.75, d^l/d^s = 1.5 \} \); (e) Larger size ratio case \( \{ H/d_0 = 60, \theta = 20^\circ, c^1_0 = 0.5, d^l/d^s = 3.0 \} \) with specifically fitted \( \sigma_{\text{seg}}^p = 0.65 \). For each case, the first column shows spatiotemporal contours of the evolution of \( c^l \) measured in the DEM simulations. The second column shows comparisons of the DEM simulations (solid lines) and continuum model predictions (dashed lines) of the \( c^l \) field at four time snapshots representing different stages of segregation: \( \tilde{t} = 2 \times 10^2, 2 \times 10^3, 1 \times 10^4 \) and \( 2 \times 10^4 \) in the sequence of top left, top right, bottom left, bottom right. The third column shows comparisons of the simulated and predicted quasi-steady, normalized velocity profiles at \( \tilde{t} = 2 \times 10^4 \).

and top. The initial concentration field is extracted from the initial DEM configuration for each case.

We then compare continuum model predictions against DEM data in the four cases of inclined plane flow discussed above – (1) base case, (2) lower inclination angle, (3) thinner layer, and (4) more large grains – as a partial validation of the model. Figures 4.12(a)-(d) summarize the comparisons and are organized in the same manner as Figs. 4.8 and 4.9. The predictions of the continuum model with the addition of the pressure-gradient-driven segregation flux term match well with DEM measurements for inclined plane flow for both the segregation dynamics and the quasi-steady flow field\(^3\) in all cases. Notably,

\(^3\)A no slip boundary condition \( v_x = 0 \) is enforced at the rough bottom in the continuum model predictions. However, it is unavoidable to have some slip at the base in the DEM simulations. In order to compare velocity profiles, the DEM velocity profile is shifted to have zero velocity at \( z = H \).
the model gives excellent predictions of the evolution of the $c^1$ field in spite of the comparatively noisier data of Fig. 4.11. We also note that for the layer thicknesses and inclination angles considered here, the NGF model plays a smaller role than in vertical chute flow or annular shear flow. Indeed, the predicted velocity fields in Fig. 4.12 are quite close to the Bagnold-type profile predicted by the local inertial rheology. For completeness, we have also included continuum model predictions and comparisons to DEM data for a higher grain-size-ratio of $d^l/d^s = 3.0$ using $C_{seg}^P = 0.65$ in Fig. 4.12(e), illustrating that the pressure-gradient-driven segregation flux involves additional dependence on the size-ratio.

## 4.8 Planar shear flow with gravity

The continuum model is now equipped to predict size-segregation phenomena involving both pressure-gradient-driven and shear-rate-gradient-driven segregation mechanisms. As a final test of the model, we consider another widely-studied quasi-one-dimensional flow configuration – planar shear flow with gravity, as discussed in Chapter 3.4.1 for the monodisperse case. Consider a dense, bidisperse granular mixture between two rough parallel walls, separated by a distance $H$. The top wall moves in the $x$-direction with a velocity $v_w$, while the bottom wall remains fixed. The top wall imposes a compressive normal stress $P_w$, and the gravitational body force $\phi \rho_s G$ acts along the $z$-direction. Periodic boundary conditions are employed along the $x$-direction, and the length of the region in the $x$-direction is $L = 60 \tilde{d}_0$, where $\tilde{d}_0$ is the system-wide average grain size. The DEM set-up is shown in Fig. 4.13(a) for $H = 120 \tilde{d}_0$, which is sufficiently large so that it does not affect flow and segregation fields and is used in all subsequently-considered cases.
The statically-determinate stress field in planar shear flow with gravity is

\[ \tau(z) = \tau_w \]

\[ P(z) = P_w + \phi \rho_s G z \]  

(4.27)

\[ \mu(z) = \frac{\tau(z)}{P(z)} = \frac{\mu_w}{1 + z/\ell}. \]

where \( \mu_w = \tau_w/P_w \) is the maximum value of \( \mu \), occurring at the wall \( (z = 0) \), and \( \ell = P_w/\phi \rho_s G \) is the loading length-scale, which is defined as the ratio of the wall pressure to the gravitational body force and is distinct from the dimensions \( H \) and \( L \). As in annular shear flow, \( \tau_w \) and hence \( \mu_w \) are not directly prescribed in our DEM simulations. The top-wall velocity \( v_w \) is prescribed with \( \tau_w \) and \( \mu_w \) arising as a result. The four important dimensionless parameters that describe planar shear flow of dense bidisperse granular mixtures with gravity are (1) \( \ell/\bar{d}_0 \), the dimensionless loading length-scale; (2) \( \bar{v}_w = (v_w/\ell)\sqrt{\pi \rho_s \bar{d}_0^2/(4P_w)} \), the dimensionless top-wall velocity, which determines \( \tau_w \) and \( \mu_w \); (3) \( c_l^0(z) \), the initial large-grain concentration field; and (4) \( d^l/d^s \), the bidisperse grain-size ratio.

The remainder of the analysis follows the process of the preceding sections. We consider a base case of quasi-static planar shear flow with gravity identified by the following parameter set: \( \{ \ell/\bar{d}_0 = 60, \bar{v}_w = 0.02, c_l^0 = 0.5, d^l/d^s = 1.5 \} \). The well-mixed initial configuration for the base-case DEM simulation is shown in Fig. 4.13(a), and the segregated configuration after a total time of \( \bar{t} = t/(\ell/v_w) = 2289 \) is shown in Fig. 4.13(b). Contours of the coarse-grained concentration field \( c_l^1 \) and the normalized velocity field \( v_x/v_w \) are shown in Figs. 4.13(c) and (d), illustrating the time-evolution of these fields. Finally, snapshots of spatial profiles of these fields at selected times – \( \bar{t} = 20, 200, \) and 2000 – are shown in Figs. 4.13(e) and (f). We observe that large grains segregate in a band just underneath the top wall with a band of small grains beneath and a persistently well-mixed base of grains. Note that since the shear-rate decreases with \( z \) and the pressure increases with \( z \), both segregation fluxes act along the same direction, and at this point, the respective contributions of
Figure 4.13: (a) Initial well-mixed configuration for two-dimensional DEM simulation of bidisperse planar shear flow with gravity with 8701 flowing grains. Black grains represent rough walls. (b) Segregated configuration after flowing for a total time of \( \tilde{t} = t/(\ell/v_w) = 2289 \). (c) & (d) Spatiotemporal evolution of the large grain concentration \( c^l \) and normalized velocity field \( v_x/v_w \), respectively. (e) & (f) Spatial profiles of concentration and normalized velocity at three times – \( \tilde{t} = 20, 200 \) and 2000 – as indicated by the dashed lines in (c) & (d).
the two mechanisms is unclear. For this reason, planar shear flow with gravity would have been a poor configuration for determining the forms of constitutive equations and fitting material parameters but is an excellent configuration for model validation.

Again, at sufficiently long time, a quasi-steady-state is reached, implying that the fluxes approximately balance as given in (4.26). We spatially coarse-grain the DEM data for 148 evenly-distributed snapshots in the quasi-steady regime ($\tilde{t} \gtrsim 1600$) to obtain all field quantities in (4.26) and then time-average these fields (before taking spatial derivatives). As previously noted, unlike in inclined plane flow, both segregation mechanisms act in the same direction. We compare the magnitudes of the two segregation fluxes (4.23) at each point in space, revealing that the shear-rate-gradient-driven segregation flux dominates the pressure-gradient-driven flux. That is to say, the right-hand-side of the flux balance equation (4.26) for planar shear flow with gravity is negligible compared to the magnitudes of the terms on the left-hand-side. This is because flow decays rapidly in planar shear flow with gravity, giving rise to strong shear-strain-rate-gradients – a feature not present in inclined plane flow. With this in mind, we plot $C_{\text{diff}} \bar{d}^2 \dot{\gamma} (\partial c^l/\partial z) + C_{\text{seg}}^P (\bar{d}^2 \dot{\gamma}/P) c^l (1 - c^l) (\partial P/\partial z)$ versus $\bar{d}^2 c^l (1 - c^l) (\partial \dot{\gamma}/\partial z)$ in Fig. 4.14 with each point representing a unique $z$-position, so that the relation is expected to be linear with a slope of $C_{\text{seg}}^S$. The process is repeated for three additional cases: (1) a lower top-wall velocity $\{\ell/\bar{d}_0 = 60, \tilde{v}_w = 0.002, c^l_0 = 0.5, d^l/d^s = 1.5\}$; (2) a smaller loading length-scale $\{\ell/\bar{d}_0 = 40, \tilde{v}_w = 0.02, c^l_0 = 0.5, d^l/d^s = 1.5\}$; and (3) more large grains $\{\ell/\bar{d}_0 = 60, \tilde{v}_w = 0.02, c^l_0 = 0.75, d^l/d^s = 1.5\}$, and the coarse-grained, quasi-steady fields are included in the data plotted in Fig. 4.14. Indeed, we observe a collapse to a linear relation with the slope of $C_{\text{seg}}^S$. The process is repeated for three additional cases: (1) a lower top-wall velocity $\{\ell/\bar{d}_0 = 60, \tilde{v}_w = 0.002, c^l_0 = 0.5, d^l/d^s = 1.5\}$; (2) a smaller loading length-scale $\{\ell/\bar{d}_0 = 40, \tilde{v}_w = 0.02, c^l_0 = 0.5, d^l/d^s = 1.5\}$; and (3) more large grains $\{\ell/\bar{d}_0 = 60, \tilde{v}_w = 0.02, c^l_0 = 0.75, d^l/d^s = 1.5\}$, and the coarse-grained, quasi-steady fields are included in the data plotted in Fig. 4.14. Indeed, we observe a collapse to a linear relation with the slope of the linear relation (indicated by the solid line in Fig. 4.14) consistent with the previously-fitted value of the dimensionless material parameter, $C_{\text{seg}}^S = 0.23$.

We then obtain predictions of the transient evolution of the segregation and flow fields using the coupled, continuum model and a fixed set of material parameters for disks with a size ratio of $d^l/d^s = 1.5 - \{\mu_s = 0.272, b = 1.168, A = 0.9, C_{\text{diff}} = 0.20, C_{\text{seg}}^S = 0.23, C_{\text{seg}}^P =$
Figure 4.14: Collapse of $C_{\text{diff}}d^2\gamma(\partial c^1/\partial z) + C_{\text{seg}}^P (d^2\gamma/P)c^1(1-c^1)(\partial P/\partial z)$ versus $d^2c^1(1-c^1)(\partial \gamma/\partial z)$ for several cases of planar shear flow of bidisperse disks with gravity with a grain-size ratio of $d_l/d_s = 1.5$. Symbols represent coarse-grained, quasi-steady DEM field data, and the solid line is the best linear fit using $C_{\text{seg}}^S = 0.23$.

0.35}. As described in Section 4.5.1 for vertical chute flow, we utilize Dirichlet fluidity boundary conditions and no flux boundary conditions at the rough walls – $z = 0$ and $z = H$. The initial concentration field is extracted from the initial DEM configuration for each case. In continuum simulations, the input value of $\mu_w$ is iteratively adjusted to achieve the target value of $\nu_w$ in the predicted quasi-steady flow field.

Comparing transient model predictions of segregation dynamics and flow with DEM measurements for the four cases of planar shear flow with gravity – (1) base case, (2) lower top-wall velocity, (3) smaller loading length-scale, and (4) more large grains – good agreement is observed, as shown in Figs. 4.15(a) through (d). The coupled continuum model prediction for a larger size-ratio of $d_l/d_s = 3.0$ is shown in Fig. 4.15(e), obtained using $C_{\text{seg}}^P = 0.65$, which also displays good agreement. We emphasize that the continuum model gives good predictions of which segregation mechanism is dominant without supposing any information beforehand. This highlights the importance of studying size-segregation in a diversity of flow configurations – rather than focusing on a single configuration as is often done in the literature [96, 98, 103].
Driven flux. Then, we re-incorporated the pressure-gradient-driven segregation mechanism and flow field. In our approach, we first focused on the shear-rate-gradient-driven size-segregation mechanism in two configurations in which the pressure field is uniform – vertical chute flow and annular shear flow – and based on observations from DEM simulations, we proposed a phenomenological constitutive equation for the shear-rate-gradient-driven flux. Then, we re-incorporated the pressure-gradient-driven segregation mechanism.

4.9 Discussion and Conclusion

In this chapter, we have studied coupled size-segregation and flow in two-dimensional, bidisperse, dense granular systems in four different configurations and developed a phenomenological continuum model that captures the simultaneous evolution of both segregation and flow fields. In our approach, we first focused on the shear-rate-gradient-driven size-segregation mechanism in two configurations in which the pressure field is uniform – vertical chute flow and annular shear flow – and based on observations from DEM simulations, we proposed a phenomenological constitutive equation for the shear-rate-gradient-driven flux. Then, we re-incorporated the pressure-gradient-driven segregation mechanism.
using two additional configurations – inclined plane flow and planar shear flow with gravity – and similarly proposed a phenomenological constitutive equation for the segregation flux driven by this mechanism. Importantly, the coupled model correctly predicts the segregation direction due to disparate particle sizes in dense granular flows: small grains tend to segregate towards regions of lower shear-strain-rate and higher pressure and vice versa for large grains. The segregation model involves three dimensionless parameters \( \{C_{\text{diff}}, C_{\text{seg}}^S, C_{\text{seg}}^P\} \) which multiply the three fluxes appearing in the model – diffusion, shear-rate-gradient-driven, and pressure-gradient-driven fluxes, respectively. By coupling the segregation model with the NGF model adapted to bidisperse systems, we may quantitatively predict both the flow fields and the segregation dynamics for dense flows of bidisperse disks, without requiring any flow field quantity input. Notably, the coupled model is
Figure 4.16: Collapse of $C_{\text{diff}} \hat{\gamma} (\partial c^l / \partial x_i)$ versus $\hat{d}_2 (\partial^l (1 - c^l) (\partial g / \partial x_i))$ for several cases of (a) vertical chute flow and (b) annular shear flow of bidisperse disks. Collapse of $C_{\text{diff}} \hat{\gamma} (\partial c^l / \partial x_i)$ versus $\sqrt{\rho_s / \hat{P} d c^l (1 - c^l) (\partial T / \partial x_i)}$ for several cases of (c) vertical chute flow and (d) annular shear flow of bidisperse disks. Symbols represent coarse-grained, quasi-steady DEM field data, and the solid lines represent the best linear fit using $C_{\text{seg}}^S = 0.08$ for (a) and (b) and $C_{\text{seg}}^S = 0.7$ for (c) and (d).

Size-segregation in granular materials is a complex and rich problem, so there remain many avenues for model improvement and unresolved research questions to be answered. One important outstanding question relates to the constitutive equation for the shear-rate-gradient-driven segregation flux (4.10). Although our use of a constitutive equation driven by gradients in $\hat{\gamma}$ has worked well, there are other theories in the literature based on gradients of other field quantities. In particular, Hill and coworkers [97, 103] have proposed that gradients in the kinetic stress – which is related to velocity fluctuations and hence the granular temperature – drive segregation. Since Zhang and Kamrin [64] have established...
a connection between velocity fluctuations and the granular fluidity $g$, it is possible to propose other forms for the constitutive equation for $w^S_i$ based on gradients in $g$. For example, instead of (4.10), consider the following form for the segregation flux:

$$w^S_i = C^{\text{seg}} d^2 c^l (1 - c^l) \frac{d g}{d x_i}. \quad (4.28)$$

Then, applying the quasi-steady-state condition,

$$C^{\text{diff}} d^2 \dot{\gamma} \frac{d c^l}{d x_i} \approx C^{\text{seg}} d^2 c^l (1 - c^l) \frac{d g}{d x_i}, \quad (4.29)$$

to the long-time DEM data for vertical chute flow and annular shear flow, we obtain the collapses shown in Fig. 4.16(a) and (b), respectively. The solid lines represent the best linear fit using $C^{\text{seg}} = 0.08$. The collapses are reasonable but not as strong as those shown in Figs. 4.5 and 4.7 for a segregation flux based on gradients in the shear-strain-rate, leading to our choice to work with the constitutive equation (4.10).

Additionally, we have also tested a possible constitutive equation for the segregation flux driven by gradients in the granular temperature, defined as $T = (\delta v)^2$, where $\delta v$ is the velocity fluctuation:\footnote{The definitions of the granular temperature $T$ and the velocity fluctuation $\delta v$ as well as the coarse-graining method used to obtain these quantities follow Zhang and Kamrin [64]. They are treated as field quantities just as $\dot{\gamma}$. Following the description in [62], instantaneous $T$ at a bin is the grain area weighted summation of the square of the difference of the grain instantaneous velocity vector and the coarse-grained instantaneous velocity field at that grain center, for all grains that are intersected by this bin.}

Then, consider the following form for the segregation flux:

$$w^S_i = C^{\text{seg}} \sqrt{\rho_s / P} d c^l (1 - c^l) \frac{d T}{d x_i}, \quad (4.30)$$

where the inertial time $\bar{d} \sqrt{\rho_s / P}$ is included in the prefactor for dimensional reasons. As

\footnote{The coarse-grained values of $g$ and its gradient are obtained using the coarse-grained values of $\dot{\gamma}$ and its gradient along with $\mu$ and its gradient which are statically-determinate and therefore not determined by coarse-graining.}
above, upon applying the quasi-steady-state condition,

\[ C_{\text{diff}} \frac{d^2 \gamma}{d \gamma} \frac{\partial \tilde{c}_l}{\partial x_i} \approx C_{\text{seg}}^S \sqrt{\rho_s / P} \tilde{c}_l (1 - c_l) \frac{\partial T}{\partial x_i}, \]  

(4.31)

Figs. 4.16(c) and (d) show the collapses for granular-temperature-gradient-driven segregation for the long-time DEM data for vertical chute flow and annular shear flow, respectively. In this case, the solid lines represent the best linear fit using \( C_{\text{seg}}^S = 0.7 \). The collapse is quite good; however, in order to utilize the constitutive equation (4.30) in practice, an additional constitutive equation that gives the granular temperature field in terms of other continuum quantities – such as strain-rate, stress, and fluidity – is needed. In summary, we acknowledge that the possibility for an alternative form for the segregation flux \( w_i^S \) remains and that future work involving additional, more-complex flow configurations – e.g., heap flow or split-bottom flow – will be required to conclusively judge which constitutive equation is the most predictive.

Another question regarding the constitutive equation for the segregation flux is the \( c_l \) dependence of the pre-factor. We simply use a symmetric dependence \( c_l (1 - c_l) \), while other researchers invoke more involved expressions that depend on both \( c_l \) and \( d_l / d_s \) in a more complex manner. Besides the constitutive equation for \( w_i^S \), we have observed that the material parameter in the constitutive equation for the pressure-gradient-driven flux, \( C_{\text{seg}}^P \), is different for the two size ratios of 1.5 and 3.0 that we considered. In order to obtain a more general model, it will be necessary to determine the functional dependence of \( w_i^P \) on \( d_l / d_s \).

In order to apply the proposed continuum model in more complex flow configurations, such as heap flows or split-bottom flow, it will be necessary to extend the theory to three-dimensions. In developing a justification for a three-dimensional generalization based on first-principles continuum thermo-mechanics, several important questions will need to be answered: (1) What is the physical nature of the segregation flux? (2) Is the segregation
flux related to a dissipative or an energetic microforce? and (3) What restrictions does the second law of thermodynamics place on the segregation flux? Such a general treatment is invaluable as it will provide a firm foundation for further generalization to more complex systems, such as continuously polydisperse systems \[110,111\]. Finally, a robust numerical implementation of the complex system of coupled equations that is capable of addressing problems in general geometries is needed. Possible approaches may be based on the finite-element method – as in previous work involving the NGF model \[72\] – or the material-point method \[35,37\], which is better equipped to model flows undergoing large distortions and with evolving free surfaces, such as those arising in rotating drums.
Chapter 5

Conclusions and outlook

5.1 Concluding remarks

From both scientific and engineering perspectives, granular materials are an interesting class of materials that pose important challenges to continuum modeling. The ability to better understand and model these materials is desirable in multiple industries as well as in geophysics in order to mitigate natural disasters such as landslides. The work in this thesis addressed several critical questions related to flow, the flow threshold, and size-segregation in dense granular materials. The main conclusions and contributions are summarized in the following:

- The nonlocal granular fluidity (NGF) model was applied to steady, dense granular heap flow in channels with frictional side walls, and the model was shown to quantitatively predict all salient experimental observations, including (1) a rapidly-flowing surface layer with rate-dependent thickness; (2) a creeping bed characterized by an exponentially decaying velocity field with rate-independent decay length; and (3) the relationships between volume flow-rate, maximum velocity, and surface inclination angle.

- The flow threshold in dense granular materials demonstrates size-dependence across
three investigated configurations – planar shear flow with gravity, annular shear flow, and vertical chute flow – in which the flow threshold increases as the size of a granular medium decreases. The dynamical form of the NGF model quantitatively captures both the size-dependence of the flow threshold and steady flow fields in all three flow configurations.

- A phenomenological continuum model for size-segregation in dense flows of bidisperse disks was proposed, involving (1) a diffusion flux, (2) a shear-strain-rate-gradient-driven segregation flux, and (3) a pressure-gradient-driven segregation flux. By coupling this model with an adapted NGF model for bidisperse granular materials, we are able to quantitatively predict both flow fields and segregation dynamics simultaneously, which no previous continuum model has achieved. The continuum model was tested by comparing model predictions against DEM simulation results of dense bidisperse flow in four configurations – vertical chute flow, annular shear flow, inclined plane flow, and planar shear flow with gravity – and the model was shown to be capable of capturing the different flow and segregation fields that arise as the configuration and various input parameters are changed.

5.2 Future directions

While progress has been made, there are numerous directions for future research work. Several directions are highlighted below.

- The NGF model remains phenomenological in nature, and further work is required to elucidate its physical underpinning. Progress on this point has been made by Zhang and Kamrin [64] and Bhateja and Khakhar [65] in establishing that the fluidity $g$ has a microscopic kinematic definition that holds across a wide diversity of flow geometries. Furthermore, Zhang and Kamrin [64] showed that the constitutive equation for the flow rule – i.e., $\dot{\gamma} = g\mu$ – is consistent with both granular kinetic theory as well as
an Eyring-like transition-state-theory picture. That said, the nonlocal rheology PDE remains phenomenological, and while the NGF model has demonstrated accuracy in flow predictions and versatility across flow geometries, obtaining the constitutive equations from a bottom-up derivation is necessary to complete the picture. Such a bottom-up derivation will help to provide physical meanings for the nonlocal amplitude $A$ and the cooperativity length $\xi(\mu)$ (2.3).

- As a corollary to the previous point, additional work is needed to obtain a clearer microscopic understanding of the fluidity boundary conditions accompanying the NGF model. In this thesis, fluidity boundary conditions were chosen primarily for pragmatic reasons, and motivating the choice of fluidity boundary conditions from a physical perspective remains an open challenge. As pointed out in Chapter 3, some progress has been made on this point for dense emulsions by Mansard et al. [83], and future work of this type is needed for dense granular materials.

As a specific class of boundary condition, the boundary between a dense, flowing granular material and a smooth frictional wall remains challenging – yet very important from a practical perspective. In the heap flow work of Chapter 2, the friction coefficient between the granular material and the side walls was taken to be a constant, which is a point worth further investigation. The work of Artoni and Richard [75] has demonstrated a dependence of the wall shear stress on the slip velocity and the velocity fluctuation – suggesting the possibility of a boundary condition in which the wall friction coefficient is dependent on both the slip velocity and the granular fluidity.

- In the quasi-static flow regime, the notion of Reynolds dilatancy – in which transient volumetric dilatation or compaction can occur during flow initiation – is well-appreciated. Volume change in the context of Reynolds dilatancy depends upon the initial preparation, and constitutive equations capable of quantitatively capturing this
phenomenology have been proposed in the context of local constitutive equations [e.g., 112, 113]. In order to obtain a more general nonlocal model, future work is needed to incorporate constitutive equations that account for Reynolds dilatancy, the associated shear strengthening/weakening, and the effect of the initial state into the NGF model.

- Concerning the continuum model for size-segregation, we have taken the segregation flux to be driven by gradients in the shear-strain-rate $\dot{\gamma}$, but potentially, gradients in other shear-related quantities could drive this flux. In our DEM tests, the form based on $\dot{\gamma}$-gradients captures DEM data best, but other candidates remain possible – such as the granular fluidity or the granular temperature. Since other works in the literature are based on the closely-related notion of kinetic stress [97, 98, 103], these forms are worth further investigation in additional flow geometries. Another issue is the $c^l$-dependence of the prefactors in the segregation fluxes. In this thesis, we used a simple symmetric form, $c^l(1 - c^l)$, in both equations (4.11) and (4.22), but more complex forms are possible [98, 109]. Furthermore, we have observed that $C^p_{seg}$ depends on the grain-size-ratio $d^l/d^s$, so it is necessary to determine the functional form of $C^p_{seg}(d^l/d^s)$ as a next step in order to obtain a more general size-segregation model.

- We have focused our segregation modeling work on quasi-one-dimensional flow configurations. The eventual goal of our continuum modeling of flow and size-segregation relates to general, three-dimensional flow settings. To achieve this, a justification based on first-principles continuum thermo-mechanics – as was done for the NGF model [60] – for the coupled model for segregation and flow is necessary. Then, implementing the three-dimensional model, which involves a system of highly coupled PDEs, in a finite-element-method or material-point-method framework presents an additional, numerical challenge.
• In this thesis, we have focused on segregation due to differences in grain size. Segregation also occurs due to mismatches in other quantities, such as density differences \cite{99} or differences in the surface friction coefficient \cite{114}, and additional modeling work will be necessary to develop constitutive equations for these mechanisms.

• Finally, granular materials exist in vast and diverse combinations of forms. In this thesis, we have focused attention on monodisperse and bidisperse mixtures of dry, stiff, spherical particles. Extending continuum models for dense granular materials to account for polydispersity \cite{115}, soft particles \cite{61-63}, various grain shapes and orientations \cite{116-118}, and pore fluid effects \cite{4,119} remains a long-term goal in granular materials modeling.
Appendix A

Technical details of DEM in LAMMPS

The DEM simulations described in this thesis were carried out using the open-source molecular dynamics (MD) code LAMMPS [79]. Molecular dynamics is a computational method widely used to study the physical movements of atoms and molecules, and with properly defined particle shapes and interaction models, it can be used to model a granular system. This appendix provides some technical details of the DEM simulations executed in this thesis.

- The built-in pair style “gran/hooke/history” – a standard Hookean spring-dashpot grain interaction model – is utilized. Interactions between grains occur only when grains overlap. The normal force consists of two terms, a repulsive elastic contact force and a damping force. The tangential force can consist of elastic and damping terms, but damping in the tangential force is turned off in our simulations. The tangential force is limited by Coulomb friction with a friction coefficient $\mu_{\text{surf}}$, and typically, the tangential force is dominated by friction.

- The microcanonical ensemble NVE is utilized, in which the total number of grains $N$, the system volume $V$, and the total energy $E$ are conserved.

- A slight polydispersity (10% or 20%) in grain-size is always included for each species.
of flowing grains. This is common practice in DEM simulations to prevent a collection of particles of the exact same size from crystallizing.

- In LAMMPS, granular particles are modeled as spheres in three-dimensions. For our purposes of modeling two-dimensional granular systems, one layer of spherical grains, all lying in the same plane, is utilized. All displacements and velocities in the out-of-plane direction are constrained, and particles only rotate about the out-of-plane direction. Thus, all contacts and motion only occur within the plane, and we discuss all simulation results in this two-dimensional plane. For example, in bidisperse mixtures, the three-dimensional densities of the two species actually need to be different in order for them to have the same area density – i.e., \( \rho_{2D} = \frac{2}{3} \rho_{3D} \). One drawback to this approach is that the mass moment of inertia for in-plane rotation of spheres and disks is different. However, this effect appears to be negligible, since the inertial rheology for disks and spheres confined to a plane are indistinguishable (see Fig. 3.2(b)).
Appendix B

Averaging method – coarse graining

Coarse-graining refers to the micro-to-macro mapping method [104] utilized to extract continuum fields from discrete DEM data. In this appendix, we briefly summarize the coarse-graining techniques utilized in this thesis.

B.1 Slices technique

First, we introduce the spatial averaging method used to obtain steady, continuum velocity and stress fields from the monodisperse DEM simulations of Chapter 3. The method follows the work of Koval and coworkers [41, 78] and is described for the cases of planar shear flow and planar shear flow with gravity, in which quantities are averaged over the x-coordinate shown in Figs. 3.2(a) and 3.3(a). First, for a snapshot at time $t$, we draw a horizontal line at a given $z$-position, and assign each intersected grain $i$ a weight $L_i$ defined as the length of the horizontal line passing through grain $i$. Then, with the instantaneous velocity of grain $i$ denoted as $v_i(t)$, the instantaneous velocity field is $v(z,t) = \sum_i L_i v_i(t) / \sum_i L_i$. Regarding the stress field, the instantaneous stress tensor associated with grain $i$ is $\sigma_i(t) = (\sum_{j \neq i} r_{ij} \otimes f_{ij}) / a_i$, where $r_{ij}$ is the position vector from the center of grain $i$ to the center of grain $j$, $f_{ij}$ is the contact force applied on grain $i$ by grain $j$, and $a_i = \pi d_i^2 / 4$ is the area of grain $i$. The instantaneous stress field follows as $\sigma(z,t) = \sum_i L_i \sigma_i(t) / L$, where $L$ is the
total length of the domain in the $x$-direction. The instantaneous velocity and stress fields are then arithmetically averaged in time over many snapshots to obtain steady fields that only depend upon the $z$-coordinate, such as those shown in Fig. 3.3(d). This process may be adapted to spatial averaging over the angular coordinate in a polar coordinate system, as described in Appendix B of Koval et al. [41], and used to obtain steady fields in annular shear flow, such as those shown in Fig. 3.4(d).

**B.2 Sliding bins technique**

The slices technique works well for velocity and stress fields. However, as shown by Weinhardt et al. [68], applying techniques of this type – i.e., ones with small or zero width in the $z$-direction – to the solid area fraction field $\phi$ will lead to spatial fluctuations due to particle-layering near walls. Since the concentration field $c^l$ is defined through the solid area fraction, we utilize an alternate bin-based coarse-graining process to obtain continuum quantities from DEM data in Chapter 4.

For specificity, we continue to consider two-dimensional flows that vary in the $z$-direction and are periodic in the $x$-direction – such as planar shear flow or planar shear flow with gravity – and discuss a process that maybe adapted to spatial averaging over the angular coordinate in a polar coordinate system. We draw a horizontal bin – i.e., a slender rectangle that spans the simulation domain along the $x$-direction – centered at a given $z$-position and with a finite width in the $z$-direction. Then, instead of defining the weight for a given intersected grain $i$ through a length, the weight is defined as the area of the intercepted grain inside the bin $A_i$. Following Tunuguntla et al. [93] for a bidisperse system, denote the sets of large and small grains intersected by a bin as $F^l$ and $F^s$, respectively, so that the set of all grains intersected by a bin is $F = F^l \cup F^s$ with $F^l \cap F^s = \emptyset$. The instantaneous solid area fraction field for species $\alpha$ is $\phi^\alpha(z,t) = (\sum_{i \in F^\alpha A_i})/A$, where $A$ is the total area of the bin, and the corresponding concentration field for species $\alpha$ is $c^\alpha(z,t) = \phi^\alpha(z,t)/\phi(z,t)$.
with \( \phi(z,t) = \phi^l(z,t) + \phi^s(z,t) \). Then, for consistency, the instantaneous velocity and stress fields are defined as \( v(z,t) = (\sum_{i \in \mathcal{F}} A_i v_i(t)) / (\sum_{i \in \mathcal{F}} A_i) \) and \( \sigma(z,t) = (\sum_{i \in \mathcal{F}} A_i \sigma_i(t)) / A^l \).

Depending on the desired spatial resolution for the coarse-grained fields and the selected bin width, adjacent bins may overlap – hence the name “sliding bins.” The sliding bins coarse-graining technique is utilized throughout Chapter 4 since our analysis of the size-segregation process depends on accurately obtaining \( c^l \) (and hence \( \phi^l \) and \( \phi^s \)) fields. Throughout, we take a bin width of \( 4d_0 \) and a spatial resolution of roughly \( 0.1d_0 \). This bin-width is sufficiently small so that the coarse-grained data is not over-smoothed but sufficiently large so that layering effects are not observed in the solid area fraction and concentration fields – i.e., we are in the plateau range [68] of bin-widths that produce bin-width-independent continuum fields. We note that in the limit that the bin-width goes to zero, we recover the slice-based coarse-graining process of Section B.1 and we have tested that over a range of bin widths – between 0 and 9.6\( d_0 \) – the coarse-grained velocity and stress fields are very similar. For a given snapshot of a DEM configuration, we start with a boundary bin centered \( 0.5d_0 \) inward from the outermost flowing grain, which means that the first few boundary bins contain empty area outside of the flowing region and are thus less accurate. We remove this wall effect by deleting coarse-grained results near walls and free surfaces. Specifically, when plotting the \( c^l \) and \( v \) profiles and contours in Chapter 4, coarse-grained data from bins centered within one-half of a bin-width (\( 2d_0 \)) from the outermost flowing grain are omitted at all walls and free surfaces. The DEM data collapses used to best fit the dimensionless material parameters \( C_{seg}^S \) and \( C_{seg}^P \) (Figs. 4.5, 4.7, 4.11 and 4.14) are more sensitive to wall effects, and therefore in these figures, we do not include spatial positions within \( 6d_0 \) of walls or free surfaces.

Unlike for the steady flows of Chapter 3 which allowed for arithmetic time-averaging as described in Section B.1 the flows of Chapter 4 involve transient, evolving fields due
to the dynamics of the segregation process. In these cases, time-averaging is performed by applying a normalized, cutoff Gaussian time filter to the DEM data at each \( z \)-position – i.e., for each bin. Denote the Gaussian standard deviation as \( \sigma_t \), so that the cutoff time-width of the Gaussian kernel is \( 6\sigma_t \). The time-smoothed field quantity at a given \( z \)-position and time \( t \) is then the convolution of the DEM data over a time-period of \( 6\sigma_t \), centered at time \( t \) – i.e., for times from \((t - 3\sigma_t)\) to \((t + 3\sigma_t)\) – with the cutoff Gaussian kernel. Concerning the choice of Gaussian time kernel width, we take \( \sigma_t \approx 6156d^8\sqrt{\rho_s/P_w} \) (or for our choice of normal contact stiffness \( k_n \) and coefficient of restitution \( e \), \( 2.8 \times 10^5\tau_c \), where \( \tau_c \) is the binary collision time) for vertical chute flow and \( \sigma_t \approx 334\sqrt{d^8/G} \) (or \( 6 \times 10^4\tau_c \)) for inclined plane flow\(^2\) For the two boundary driven flows, \( \sigma_t \) varies across cases to maintain the boundary shearing displacement inside the kernel time-width roughly equal for each case for a given flow configuration. For the width of a Gaussian time filter, each annular shear flow case has an inner-wall tangential displacement of \( \sim 2000\bar{d}_0 \), and the top-wall shearing displacement for each planar shear flow with gravity case is \( \sim 8000\bar{d}_0 \). (This distinction between the two configurations is due to the different wall displacements needed to achieve a quasi-steady segregated state.) Finally, we note that our coarse-grained continuum fields are relatively consistent for changes in Gaussian time kernel widths within the tested ranges – i.e., \( \sigma_t \in (2638d^8\sqrt{\rho_s/P_w}, 9674d^8\sqrt{\rho_s/P_w}) \) for vertical chute flow and \( (200\sqrt{d^8/G}, 600\sqrt{d^8/G}) \) for annular shear flow and kernel times corresponding to wall shear-displacements in \((1000\bar{d}_0, 2600\bar{d}_0)\) for annular shear flow and \((3500\bar{d}_0, 12500\bar{d}_0)\) for linear shear flow with gravity.

The collapses of Figs. 4.5, 4.7, 4.11 and 4.14 are obtained in the long-time regime, in which the fields evolve slowly in time. Since the flow is quasi-steady, instead of subjecting the DEM data to time filtering as described in the previous paragraph, the velocity and concentration fields are simply arithmetically averaged in time to obtain fields that only

\(^2\)The binary collision time \( \tau_c \) was defined for monodisperse systems in Chapter 3.2.1 and for bidisperse mixtures, it is defined as \( \tau_c = \sqrt{\pi\rho_s\bar{d}_0^2(\pi^2 + \ln^2(e))}/16k_n \). The DEM time step is chosen as 0.1 of \( \tau_c \) for vertical chute flow and 0.03 of \( \tau_c \) for annular shear flow, inclined plane flow, and planar shear flow with gravity of bidisperse disks to ensure stable simulation results while balancing computation time.
depend on the spatial coordinate. Then, the necessary first and second-order spatial derivatives of the field quantities – i.e., $\partial c^i/\partial z$, $\dot{\gamma} = \partial v/\partial z$, and $\partial \dot{\gamma}/\partial z = \partial^2 v/\partial z^2$ – are obtained from these time-averaged fields. Instead of using a finite-difference-based approach, we apply a Gaussian spatial derivative filter to the time-averaged data in order to obtain better accuracy and more spatial smoothing. This approach is possible because the derivative of the convolution of a signal and a kernel is equal to convolving the signal with the derivative of the kernel. The standard deviation of the Gaussian spatial derivative filter $\sigma_s = 0.5 \bar{d}_0$ throughout, which leads to a filter width of 30 bins.

As a final comment, other works in the literature [68, 104] have focused on choosing appropriate filter functions – e.g., Lucy functions instead of Gaussian functions – and coarse-graining widths. Although we have not exhaustively studied the effects of coarse-graining widths, we have been careful to ensure that the reported results in Chapter 4 are independent of these choices. Future work will focus on developing more systematic criteria for selecting coarse-graining time and space scales for problems involving size-segregation.
Appendix C

Diffusion flux consistency check

Our process for determining the segregation flux – and hence the material parameters $C_{seg}^{S}$ and $C_{seg}^{P}$ – is based on the assumption that the segregation and diffusion fluxes balance in the quasi-steady regime. Therefore, it is essential that the dimensionless material parameter $C_{diff}$ appearing in the constitutive equation for the diffusion flux (4.9) has been accurately determined, so that the coarse-grained diffusion flux is accurate. In Section 4.3, we determined $C_{diff}$ for disks to be 0.20 using mean square displacement data from DEM simulations of planar shear of a well-mixed bidisperse granular system. In this appendix, we perform an independent consistency check that tests whether the constitutive equation for the diffusion flux (4.9) using this fitted $C_{diff}$ value is capable of predicting the evolution of the $c^l$ field in a diffusion-dominated problem.

Consider homogeneous planar shear flow of an initially-segregated system with large grains on the bottom and small grains on the top, as shown in Fig. C.1(a). We run the DEM simulation starting from the initially-segregated configuration, and the spatiotemporal evolution of the coarse-grained $c^l$-field is shown in Fig. C.1(b). We observe that the interface between large and small grains, which is initially sharp, becomes diffuse with a transition width that grows with time. We define a transition width at a given point in time as the distance between the points where $c^l$ equals 0.1 and 0.9 in snapshots of the spatial $c^l$ profile.
This transition width as a function of the square-root of time is plotted in Fig. C.1(c) as solid lines for grain-size-ratios of $d^1/d^5 = 1.5$ and $3.0$, displaying roughly linear behavior – typical of diffusive behavior – with a slight dependence on $d^1/d^5$.

Next, we apply the continuum model for the evolution of $c^1$ (4.11) to this problem. As
for planar shear flow of a monodisperse granular system (Fig. 3.2) or a well-mixed bidisperse system (Fig. 4.2), no pressure gradient is present, and the shear-strain-rate is approximately constant, leading to approximately zero shear-rate-gradient throughout. Therefore, the diffusion flux is the dominant flux, which acts to remix the flowing grains. The equation governing the evolution of $c^l$ (4.11) becomes

$$\frac{Dc^l}{Dt} + \frac{\partial}{\partial z} \left( -C_{\text{diff}} d^2 \dot{\gamma} \frac{\partial c^l}{\partial z} + C_{\text{seg}} d^2 c^l (1 - c^l) \frac{\partial \dot{\gamma}}{\partial z} \right) = 0,$$

(C.1)

where $\bar{d} = c^l d^l + (1 - c^l) d^s$. We note that due to the tiny effect of segregation and the dependence of $\bar{d}$ on $c^l$, (C.1) is similar to but not exactly the same as the linear diffusion equation in one dimension, so the solution is close to but not exactly an error function.

We obtain predictions for the evolution of the $c^l$-field using the fully-segregated initial condition for $c^l(z, t = 0)$, no-flux boundary conditions at $z = 0$ and $z = H$, a spatially-constant value of inertial number $I$ consistent with that prescribed in the DEM simulations, a given grain-size-ratio $d^l/d^s$, and $C_{\text{diff}} = 0.20$. We extract the transition width as a function of time from continuum simulation results for $d^l/d^s = 1.5$ and $3.0$ and include these results in Fig. C.1(c) as dashed lines. The continuum model predictions agree well with the DEM data and are even capable of capturing the small difference due to the grain-size-ratio. This result indicates that the expression for the diffusion flux (4.9) and the fitted material parameter value $C_{\text{diff}} = 0.20$ are indeed consistent with DEM data. We conclude by re-emphasizing that this test is simply a consistency check for the constitutive equation for the diffusion flux. We do not use this test to fit the value of $C_{\text{diff}}$, nor do we consider this test as validation of the model.

---

1 In the context of the local inertial rheology, since the stress ratio $\mu$ is spatially-constant in homogeneous planar shear, the resulting inertial number field $I$ is also spatially constant. Since the inertial number depends on both $d$ and $\dot{\gamma}$, spatial variation in $\bar{d}$ leads to spatial variation in $\dot{\gamma}$. Even though this spatial variation in $\dot{\gamma}$ is slight, and we still include the shear-strain-rate-gradient-driven segregation flux when analyzing the problem shown in Fig. C.1(a).

2 Note that since $I$ is taken to be spatially-constant, $\dot{\gamma} = (I/\bar{d}) \sqrt{F_w/\rho}$ varies slightly in space due to the $c^l$-dependence of $\bar{d}$. 
Bibliography


