

THE SIMULATION AND MODELING OF SETTLING AND CLUSTERING
BEHAVIOR OF POLYDISPERSE GAS-SOLID FLOWS WITH APPLICATION TO
PYROCLASTIC DENSITY CURRENTS

by

EMILY SUSAN FOSTER

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Oakland University
Rochester, Michigan

Doctoral Advisory Committee:

Sarah Beetham, Ph.D., Chair
Christopher Cooley, Ph.D.
Laila Guessous, Ph.D.
Osamah Rawashdeh, Ph.D.
Xia Wang, Ph.D.

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For the women still climbing.

*I stand
on the sacrifices
of a million women before me
thinking
what can I do
to make this mountain taller
so the women after me
can see farther
- Rupi Kaur*

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Emily Susan Foster

ABSTRACT

THE SIMULATION AND MODELING OF SETTLING AND CLUSTERING BEHAVIOR OF POLYDISPERSE GAS-SOLID FLOWS WITH APPLICATION TO PYROCLASTIC DENSITY CURRENTS

by

Emily Susan Foster

Adviser: Sarah Beetham, Ph.D.

Gas-solid flows are present in many industrial and natural systems, including fluidized beds, energy systems, and pyroclastic density currents (PDCs). Predicting these flows remains challenging due to complex interactions between particles and the carrier fluid, particularly in polydisperse systems where particle sizes vary significantly. These challenges are especially important for PDCs, whose large temporal and spatial scales require coarse-grained multiphase flow solvers with closure models to represent unresolved particle-scale physics. This work investigates the settling and clustering dynamics of polydisperse gas-solid flows relevant to PDCs using high-fidelity Euler-Lagrange simulations and develops models and correlations for coarse-grained solvers.

Particle size distribution effects were examined across multiple volume fractions and compared to equivalent monodisperse systems. Smaller particles were found to occupy voids within particle assemblies, increasing clustering intensity and settling

velocity, while existing predictors based on volume fraction or isolated particle settling laws failed to represent this behavior. To address this, a new *surface loading* parameter was introduced and used to develop predictive models for particle-phase averaged fluid velocity and settling velocity. A proposed drag model accounting for clustering effects also provided improved agreement with the simulation data and accurately predicted settling behavior across particle sizes.

Because existing scaling relationships developed for monodisperse systems performed poorly for polydisperse flows, a new logarithmic scaling relationship based on modal particle diameter was established to predict the characteristic cluster length and provide an *a priori* estimate of the domain size required to obtain domain-independent statistics, accurately capturing the observed domain-size dependence.

Finally, filtering effects on particle-phase turbulent kinetic energy and granular temperature were examined. Particle size distributions were shown to significantly alter the smallest reliable filter size relative to monodisperse systems, and a new model was developed to predict the resulting unresolved granular temperature with good agreement to the simulation data.

These results provide new insight into the behavior of polydisperse gas-solid flows and improve coarse-grained multiphase flow solvers for PDCs and other particle-laden systems.

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CHAPTER 1

INTRODUCTION

Sedimenting multiphase flows occur in a wide range of society-critical applications. In industrial settings, these flows are important in systems such as circulating fluidized bed reactors, where gas–solid interactions govern the efficiency of biomass upgrading into biofuels [1, 2]. At larger scales, sediment-laden flows affect how contaminants move through groundwater aquifers [3] because particle settling, dispersion, and filtration directly affect water quality and public health. Similar processes arise in the atmosphere, where aerosols ranging from mineral dust to environmental pollutants undergo gravitational settling, turbulent mixing, and chemical transformation, altering air quality and visibility [4, 5]. Sedimenting multiphase flows also govern several high-impact natural hazards. Volcanic processes, such as column collapse, pyroclastic density currents, and ash fallout, are fundamentally controlled by particle settling dynamics and particle–gas coupling [6]. Likewise, snow avalanches and debris flows involve dense, gravity-driven mixtures whose runout, internal structure, and destructive potential depend on interactions between dispersed solids and surrounding fluids [7–10]. Across all of these contexts, particle settling, fluid turbulence, and multiphase coupling govern system behavior and are difficult to predict. In industrial settings, improved understanding enhances process efficiency and operational safety. Accurate descriptions of multiphase flow dynamics can also inform decisions such as evacuation planning,

land-use assessments, and the management of water and air quality. Understanding how these flows behave is essential for predicting hazards and minimizing risks to people, infrastructure, and the environment. This work is motivated by pyroclastic density currents (PDCs). PDCs are a hot, ground-hugging mixture of volcanic gas, ash, and rock fragments that flows rapidly downslope under the influence of gravity. These currents are generated during explosive volcanic eruptions when an eruption column collapses. Because the mixture is denser than the surrounding atmosphere, it remains close to the ground and can travel at speeds exceeding 100 m/s, over distances of tens of kilometers, with temperatures ranging from a few hundred to more than 800°C. For this reason, they are considered the most lethal volcanic process following an eruption. Over 100 million people currently live at risk from PDC hazards [6, 11, 12]. While laboratory experiments and measurements can be performed to some extent [10, 11, 13], they are often limited to coarse-grained observations or become impractical due to the costs, risks, and scales involved. As a result, computational modeling approaches are frequently used to obtain detailed information about these flows.

PDCs span a broad range of spatial and temporal scales, making direct resolution of all relevant physics computationally impractical. Consequently, a variety of multiphase modeling approaches have been developed, each balancing physical fidelity and computational cost differently [6, 14–19]. Common multiphase flow frameworks include Euler-Euler (EE) and Two-Fluid Models (TFM) [20–29], Eulerian-Lagrangian (EL) methods [30–35], and Particle-in-Cell (PIC) [36] approaches. These frameworks are often

coupled with turbulence-resolution strategies such as Direct Numerical Simulation (DNS) [37, 38], Particle-Resolved Direct Numerical Simulation (PR-DNS) [39–41], Large-Eddy Simulation (LES) [42, 43], and multiphase Reynolds-Averaged Navier-Stokes (RANS) methods. These methods differ primarily in how the dispersed particle-phase is represented and in how unresolved particle-fluid interactions are modeled. Coarse-grained and reduced-order approaches are commonly employed for large-scale simulations due to their computational efficiency. However, these methods inherently rely heavily on models and closures to represent unresolved physics, including drag, turbulence modulation, particle clustering, collisional stresses, and interphase momentum exchange [20, 44–48].

Although significant progress has been made in developing closures for such multiphase systems, closures for subgrid behavior in natural hazards remain limited, particularly for highly polydisperse flows such as PDCs. Capturing the effects of unresolved mesoscale particle structures, turbulence behavior, and particle-fluid interactions remains one of the primary challenges in developing predictive coarse-grained multiphase solvers for volcanic flows. The present work focuses on developing such modeling closures for large-grained multiphase simulations of PDCs using high-fidelity Euler-Lagrange simulations, in which collected steady-state flow statistics are used to develop physically informed closure models.

1.1 BACKGROUND AND MOTIVATION

1.1.1 WHAT ARE MULTIPHASE FLOWS?

The governing equations presented throughout this work depend on the number of phases present within the flow. A single-phase flow consists of a single continuous phase, such as a liquid or gas, and can be described using one set of governing equations. These equations are the conservation of mass and momentum, and optionally the conservation of energy when the flow is not assumed to be isothermal. In contrast, a multiphase flow involves the motion of two or more distinct phases, commonly combinations of gases, liquids, and solid particles that interact with each other. A single set of governing equations therefor are no longer sufficient to describe these flows. Instead, each phase has its own governing equations, while also accounting for the coupling of the phases. These governing equations generally consist of the conservation of mass and momentum for the continuous phase, together with additional equations describing the evolution of the dispersed phase and closure relationships governing the exchange of mass, momentum, and energy between the phases. The specific form of these equations depends on the modeling framework employed. These governing equations will be discussed in detail in the following sections.

1.1.2 CHALLENGES IN MULTIPHASE FLOW SIMULATION

Multiphase flows exhibit a range of challenging physical behaviors. Such flows involve physical processes spanning many different length scales, from individual grain sizes to

mesoscale particle clusters to the full flow height, and a wide range of time scales, from the fast dynamics of particle collisions or turbulent eddies to the slower evolution of a bulk granular flow-6. Adding to the complexity, these flows often experience particle-particle collisions and the formation of coherent structures that generate and sustain turbulence in the surrounding fluid. Further models and *a priori* predictors for particle settling velocity are widely used to estimate the rate at which particles fall through a fluid, providing a simplified framework for interpreting complex multiphase behavior. Classical formulations, such as Stokes' settling law, assume idealized conditions including isolated, spherical particles in a quiescent fluid at low Reynolds number [49–52]. While these models are useful for establishing baseline trends and scaling relationships, they neglect important physical effects such as particle–particle interactions and multiphase turbulence. As a result, they often oversimplify real systems, particularly in dense or turbulent flows where collective behavior and mesoscale structures significantly influence settling dynamics.

1.1.2.1 SINGLE AND MULTIPHASE TURBULENCE In single-phase flows, turbulence refers to fluctuations in a velocity field. In this case, the turbulence is entirely generated and sustained by the fluid itself. It is often difficult to quantify how turbulent fluctuations affect mean flow behavior. Therefore, Single-phase turbulence is often described using Reynolds decomposition. Reynolds decomposition is a mathematical technique in turbulence modeling that separates a flow variable into a mean and a

fluctuating component, allowing the effects of turbulence to be represented statistically rather than explicitly resolved [53]. In the context of turbulence, the velocity field can be decomposed into a mean and a fluctuating component as

$$\mathbf{u} = \langle \mathbf{u} \rangle + \mathbf{u}'. \quad (1.1)$$

where $\mathbf{u}$ is the instantaneous velocity vector, $\langle \mathbf{u} \rangle$ is the mean velocity vector, and $\mathbf{u}'$ represents the fluctuating velocity vector about the mean.

This method facilitates the first step in understanding turbulent single-phase flows. This decomposition can be leveraged by applying it to the governing equations describing single-phase behavior, i.e., the Navier-Stokes equations for conservation of mass and momentum [53],

$$\nabla \cdot \mathbf{u} = 0, \quad (1.2)$$

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} \nabla p + \nabla \cdot [\nu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)] + \mathbf{g}, \quad (1.3)$$

where $\mathbf{x}$ is the Cartesian position vector, t is time, p is the pressure, ρ is the fluid density, ν is the kinematic viscosity, and $\mathbf{g}$ is the gravitational acceleration vector. Here, $\nabla \mathbf{u}$ denotes the velocity gradient tensor and $(\nabla \mathbf{u})^T$ is its transpose.

Applying the decomposition to the conservation of mass and momentum (Eqs. (1.2) and (1.3)) results in the Reynolds-Averaged Navier-Stokes (RANS) equations given

by,

$$\nabla \cdot \langle \mathbf{u} \rangle = 0, \quad (1.4)$$

$$\frac{\partial \langle \mathbf{u} \rangle}{\partial t} + \langle \mathbf{u} \rangle \cdot \nabla \langle \mathbf{u} \rangle = -\frac{1}{\rho} \nabla \langle p \rangle + \nabla \cdot [\nu (\nabla \langle \mathbf{u} \rangle + (\nabla \langle \mathbf{u} \rangle)^T) - \mathbf{R}] + \mathbf{g}, \quad (1.5)$$

where $\mathbf{R} = \langle \mathbf{u}' \mathbf{u}' \rangle$ is the Reynolds stress tensor, which arises from Reynolds decomposition of the velocity field and represents the transport of momentum due to turbulent velocity fluctuations.

Non-dimensionalization of the RANS equations using characteristic velocity and length scales U and L yields key dimensionless numbers. These parameters include the Reynolds number, $Re = UL/\nu$, which quantifies the relative importance of inertial forces versus viscous forces and is used to determine whether a flow is laminar or turbulent. Another important non-dimensional number is the Froude number, $Fr = U/\sqrt{gL}$, which is the ratio of inertial to gravitational (or other external body) forces.

All the terms appearing in the RANS equations are expressed in terms of mean flow quantities, except for the Reynolds Stresses, which require modeling, as they represent unknown turbulent fluctuations. Modeling enables the approximation of these complex turbulent interactions to compute realistic mean flow behavior. The Boussinesq approximation [54] was proposed shortly after the derivation of the RANS equations. The Boussinesq approximation established a relationship between the Reynolds stresses and

the mean shear tensor, via a turbulent viscosity ν_t . This relationship is given as,

$$\mathbf{R} = -\nu_t (\nabla \langle \mathbf{u} \rangle + (\nabla \langle \mathbf{u} \rangle)^T) - \frac{2}{3}k\mathbb{I}, \quad (1.6)$$

where ν_t is the turbulent (eddy) viscosity, k is the turbulent kinetic energy, and $\mathbb{I}$ is the second-order identity tensor. The turbulent kinetic energy is defined as one-half the trace of the Reynolds stress tensor,

$$k = \frac{1}{2}\text{tr}(\mathbf{R}). \quad (1.7)$$

The Boussinesq approximation assumes that the Reynolds stresses are proportional to the mean rate of strain through an isotropic turbulent viscosity. This hypothesis forms the foundation of many eddy-viscosity turbulence models, including the k - ε and k - ω families of models [55–57].

Kolmogorov later introduced the *K41 theory* [58], which describes the transfer of turbulent kinetic energy from large to small scales. In this framework, energy is generated at large scales, such as eddies formed by vortex shedding, and is transported through an intermediate *inertial range* before being dissipated as heat at the smallest scales by viscous effects. In the *K41 theory*, turbulent energy cascades toward smaller scales following a characteristic $-5/3$ power-law scaling.

This theory also introduced the Kolmogorov length scale, η , which represents the smallest dynamically relevant turbulent length scale and is defined as

$$\eta = \left(\frac{\nu_f^3}{\varepsilon_f} \right)^{1/4}, \quad (1.8)$$

where ε_f is the turbulent kinetic energy dissipation rate and ν_f is the fluid kinematic viscosity. At length scales smaller than η , viscous forces dominate, and turbulent motions are converted into heat.

It is worth mentioning that in recent decades, researchers have shown that inverse energy transfer can also occur in single-phase flows under certain conditions [59, 60]. Although the net energy transfer in homogeneous, isotropic three-dimensional turbulence remains predominantly forward, inverse energy transfer has been observed in rotating, stratified, quasi-two-dimensional, and other anisotropic flows, highlighting that turbulence consists of competing forward and inverse transfer mechanisms rather than a purely forward cascade [59–62].

Multiphase turbulence, in contrast, occurs when turbulence develops in a flow containing more than one phase. Historically, two-phase turbulence modeling has been derived from single-phase turbulence models [63–71]. Multiphase turbulence is more complex and requires a set of governing equations for each phase. Fox [72] showed that directly averaging the Navier-Stokes equations fails to capture two-phase and particle-particle interactions. As a result, Fox [72] demonstrated that averaging the

mesoscale equations yields a mathematical formulation that accounts for two-way coupling. Capecelatro [73] expanded on this work and derived exact RANS equations for multiphase turbulent flows (discussed in greater detail in Chapter 2). In these flows, the presence of additional phases alters the fluid's turbulent motion, while turbulence, in turn, affects how particles move, settle, and cluster. Particles may enhance or hinder turbulence depending on their size, concentration, and inertia, leading to feedback between the phases that does not exist in single-phase flows. Several dimensionless groups arise when describing such flows. For a disperse phase with particulates with diameter d_p , density ρ_p , and volume fraction α_p (defined as the ratio of the volume occupied by particles to the volume of the total domain, $\sum_{i=1}^{N_p} V_p/V_{\text{domain}}$), these dimensionless numbers include particle-fluid density ratio ρ_p/ρ_f and mass loading given as $\varphi = \rho_p \langle \alpha_p \rangle / (\rho_f \langle \alpha_f \rangle)$, which can be considered as the ratio of the mass of the particles to the mass of the fluid in a given volume of the flow where the mean particle and fluid volume fractions are given as $\langle \alpha_p \rangle$ and $\langle \alpha_f \rangle$ respectively. An additional parameter that arises is the Stokes number, $St = \tau_p/\tau_\eta$, which quantifies how strongly particles are coupled to the surrounding fluid flow, particularly to its turbulent motions. Physically, it compares the response time of a particle, τ_p , to the characteristic timescale of the fluid motion it is in, τ_η , wherein $\tau_p = \rho_p d_p^2 / (18\mu_f)$, $\tau_\eta = \sqrt{\left(\frac{\nu_f}{\varepsilon_f}\right)}$, and μ_f is the fluid dynamic viscosity. When the Stokes number is low, the particles respond rapidly to fluctuations in fluid velocity and therefore behave like tracers, closely following turbulent eddies and remaining suspended in the surrounding fluid. When the Stokes number increases to around one, particles can no

longer follow the fluid's motion. Instead, they are pushed out of turbulent fluid regions and tend to cluster in calmer regions of the flow. For larger Stokes numbers, particles are largely decoupled from the turbulent flow, maintaining their own trajectories and responding weakly to turbulent fluctuations in the fluid-phase, thereby promoting rapid particle settling.

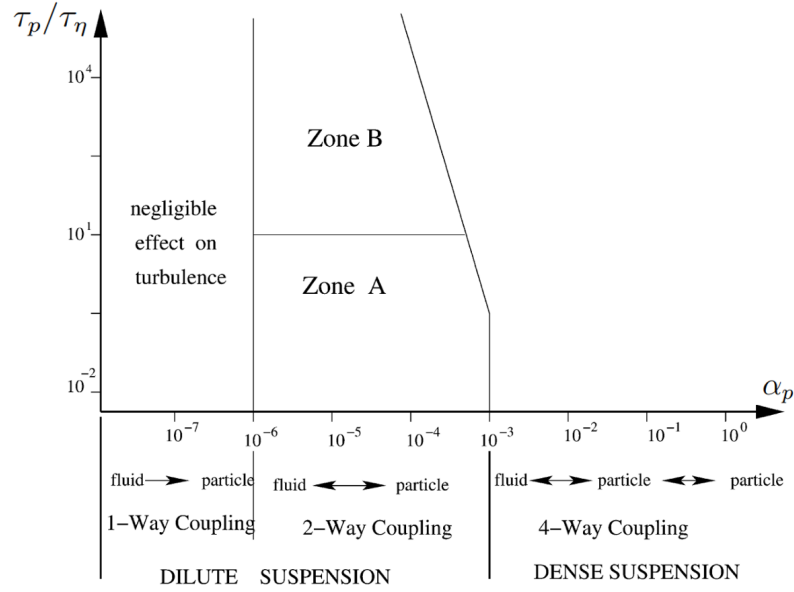


Figure 1.1: Classification map of particle-laden turbulent flows as a function of particle volume fraction, α_p , and the ratio of particle response time to Kolmogorov time scale, τ_p/τ_η . The diagram highlights regimes associated with one-way, two-way, and four-way coupling, corresponding to increasing levels of momentum exchange and particle-particle interactions within the flow. At low particle concentrations, particle effects on turbulence are negligible, whereas increasing particle loading leads to turbulence modulation and dense-suspension behavior. Adapted from [74].

A wide range of regimes are possible in multiphase flows, as shown in Figure 1.1.

Particles act as tracers in the flow when the volume fraction is low, also known as one-way coupling. As the volume fraction increases, particle interactions increase, and the fluid and particle phases affect one another. This is referred to as two-way coupling. In

this regime, the particles alter the turbulence in the neighboring fluid, and the fluid alters particle pathways. In very dense particulate suspensions, particle-particle collisions are prominent, referred to as four-way coupling. In this regime, particulates can form large coherent structures where particles begin to closely pack with each other, known herein as clusters [75]. These clusters can also alter turbulence in the neighboring fluid, a phenomenon known as cluster-induced turbulence (CIT). CIT arises from particle-scale interactions, making multiphase turbulence fundamentally different from classical single-phase turbulence. As particles preferentially concentrate into dense regions, they create localized velocity disturbances and wakes that inject energy at the cluster scale (Refer to Figure 1.2).

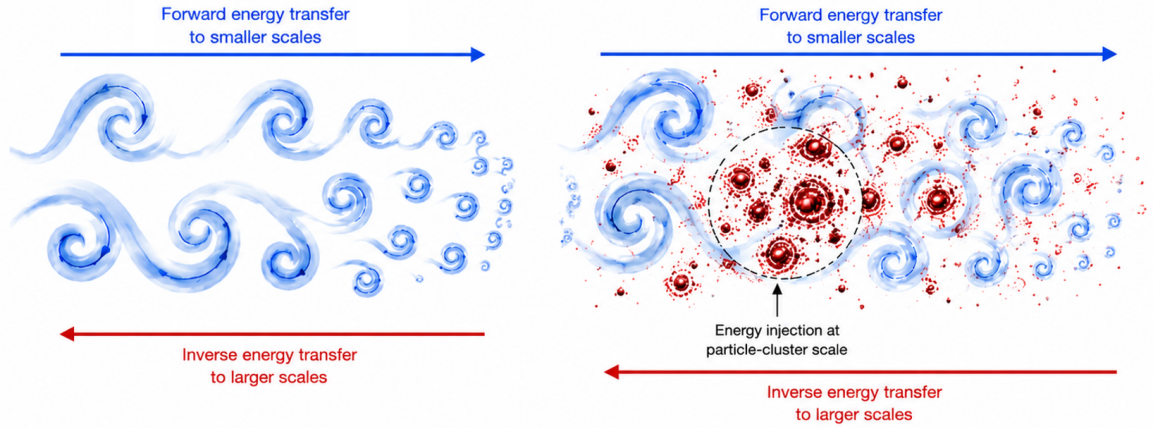


Figure 1.2: Conceptual illustration of turbulent energy transfer in single-phase (left) and particle-laden multiphase (right) flows. In single-phase turbulence, kinetic energy predominantly cascades from large to small eddies (forward cascade), while inverse energy transfer may also occur under certain flow conditions. In particle-laden flows, preferential particle clustering injects energy at the cluster scale, promoting additional inverse energy transfer and modifying the classical cascade across a range of turbulent scales. Image generated using AI-assisted visualization tools.

These disturbances subsequently organize into larger coherent flow structures through momentum exchange between the particles and the carrier fluid [76]. As a result,

CIT has become a major area of research in multiphase flow physics. Numerous experimental [77], theoretical [58], and computational investigations [41, 73, 78–85] have examined the formation of clusters, the generation of fluid-phase velocity fluctuations, turbulence modulation, particle settling, and interphase momentum exchange associated with CIT. These studies span a broad range of particle Reynolds numbers, volume fractions, density ratios, and flow configurations, demonstrating that CIT strongly influences the macroscopic behavior of particle-laden flows. Consequently, accurately capturing CIT remains a critical challenge for multiphase flow modeling and simulation. Different computational methods are employed depending on the flow regime and quantities of interest in these differing regimes (refer to Figure 1.3 for a high-level overview of computational methods).

1.1.2.2 PARTICLE-RESOLVED DIRECT NUMERICAL SIMULATION, DIRECT NUMERICAL SIMULATION, AND LARGE-EDDY SIMULATION

Among the highest-fidelity approaches for simulating multiphase flows are Particle-Resolved Direct Numerical Simulation (PR-DNS) and Direct Numerical Simulation (DNS) [39–41].

PR-DNS is a computational approach that solves the Navier-Stokes equations without turbulence modeling while explicitly resolving the flow surrounding individual particles.

The method resolves all turbulent scales while explicitly capturing particle boundary layers and wake interactions due to the presence of a dispersed phase. As a result,

PR-DNS requires extremely fine spatial and temporal resolution because the flow around

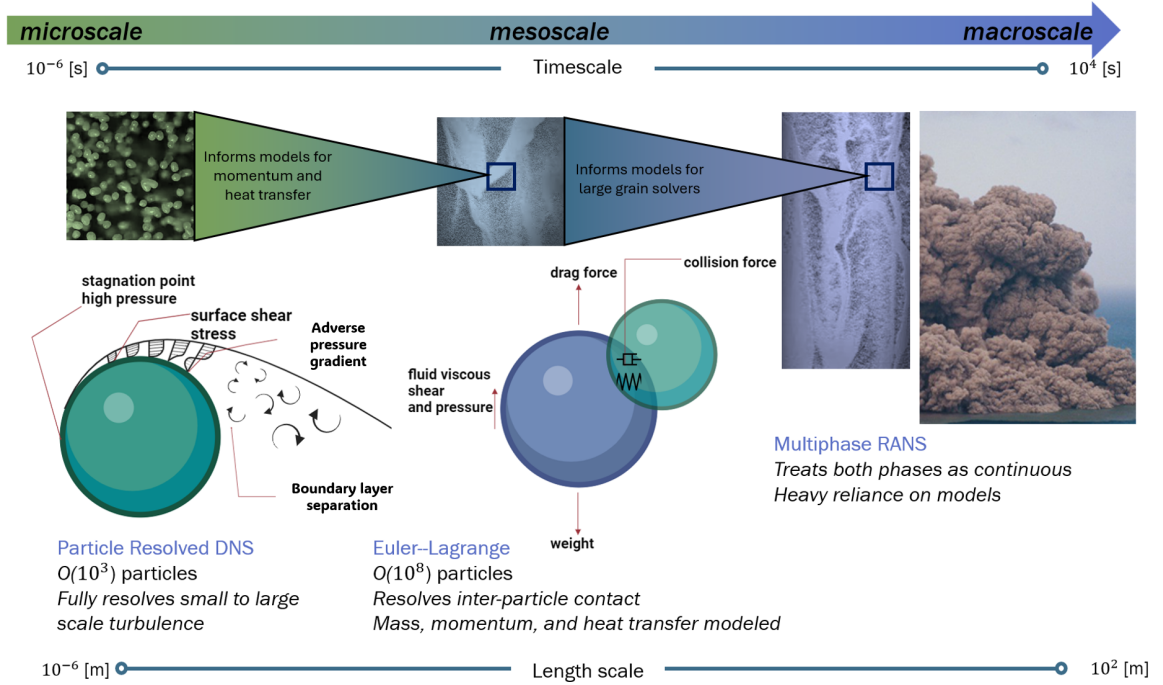


Figure 1.3: Schematic illustrating the relationship between computational modeling strategies and the physical scales encountered in particle-laden multiphase flows. PR-DNS provides high-fidelity simulations by resolving the flow surrounding individual particles, Euler-Lagrange methods resolve particle dynamics while modeling unresolved fluid-particle interactions, and multiphase RANS represents both phases as continua through averaged governing equations and empirical closures. This progression from microscale to macroscale highlights the trade-off between physical fidelity and computational cost, motivating the development of improved closure models for coarse-grained simulations. The images across the top depict the increasing physical scale from individual particles to a pyroclastic density current, with the particle images obtained from high-speed imaging of a circulating fluidized bed reactor [86].

each particle must be resolved directly. Due to the high computational cost, these

simulations are typically limited to relatively small systems containing $\mathcal{O}(10^3)$ particles.

Despite this limitation, PR-DNS can capture mesoscale behavior, such as the formation of coherent particle structures.

In contrast, DNS resolves all turbulent scales of the carrier fluid without explicitly resolving particle-scale flow structures. In multiphase applications, DNS often employs

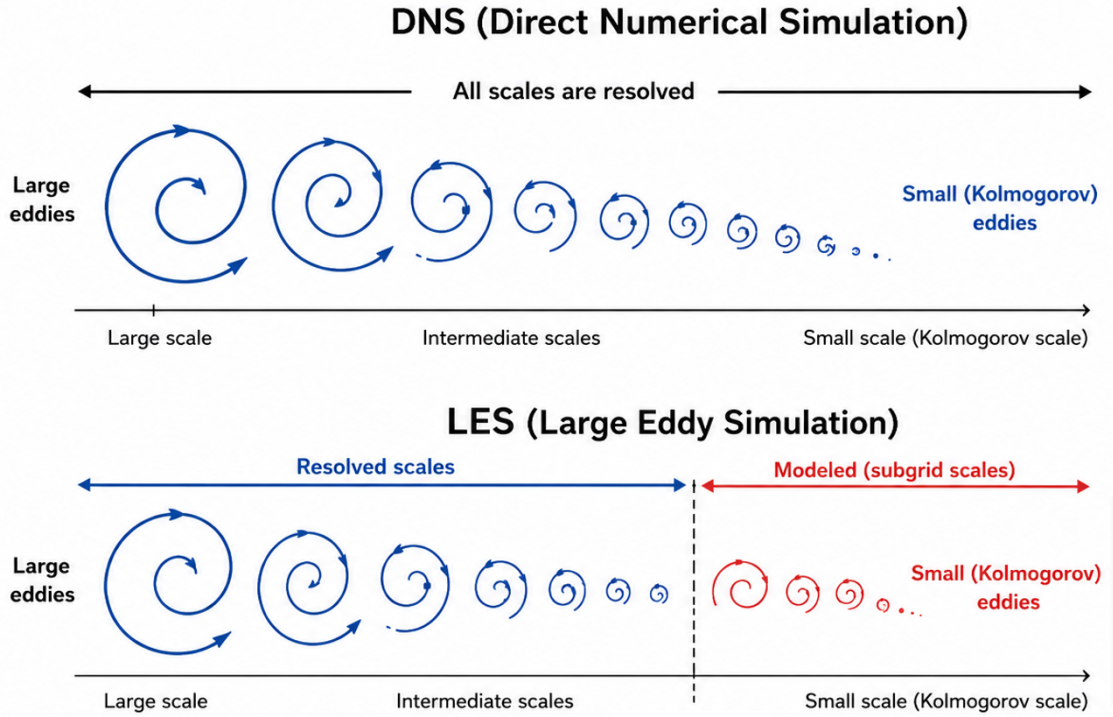


Figure 1.4: Comparison of the turbulence scales resolved in Direct Numerical Simulation (DNS) and Large Eddy Simulation (LES). DNS resolves the complete spectrum of turbulent motions, from the largest energy-containing eddies to the smallest dissipative scales. In contrast, LES directly resolves the large, energy-containing eddies while modeling the unresolved subgrid-scale motions using a turbulence closure. Image generated using AI-assisted visualization tools.

point-particle representations of the dispersed phase. Point-particle DNS approaches are most commonly applied to dilute suspensions where particle volume fractions are sufficiently low that particle-scale flow structures and interparticle collisions can be neglected. [37, 38]. LES simulation reduces the computational cost by resolving the large, energy-containing turbulent eddies while modeling the unresolved subgrid-scale turbulence[87]. Figure 1.4 shows a schematic of the resolved and unresolved turbulence scales in DNS and LES. PR-DNS, DNS, and LES can be leveraged to inform models for mesoscale multiphase behavior [42, 43].

1.1.2.3 EULERIAN-LAGRANGIAN Unlike PR-DNS, which resolves the flow surrounding every particle, Eulerian-Lagrangian (E–L) framework models particle-fluid interactions through closure relations while explicitly tracking the trajectories of individual particles. This substantially reduces the computational cost, enabling simulations with significantly larger particle populations and computational domains. Such methods have been explored extensively [30–35]. This framework resolves particle motion explicitly while relying on models for interphase drag [20, 44–47] and particle collisions [48]. This framework adopts a method in which the carrier phase is solved in an Eulerian reference frame and, in contrast, the dispersed phase is represented by discrete Lagrangian particles that are tracked individually through the flow [81, 88]. This method can simulate up to $\mathcal{O}(10^8)$ particles on average but can be computationally expensive for larger length and time scales. Within E–L framework, each particle satisfies its own equations of motion and exchanges momentum with the surrounding fluid through interphase exchange models. This framework can resolve particle-particle clustering and particle-turbulence interactions more directly than continuum approaches. Because fluid quantities are obtained from discrete particle statistics, E–L simulations generally require a sufficiently large number of computational particles to reduce statistical sampling error. Such simulations can aid the development of closures for simplified or larger-scale solvers.

1.1.2.4 EULERIAN-EULERIAN, TWO-FLUID MODELS, AND PARTICLE-IN-CELL

Accurately capturing CIT requires resolving both particle-scale interactions and the

mesoscale turbulence they generate. For large-scale multiphase systems where resolving individual particle trajectories becomes computationally expensive, Eulerian-Eulerian (E-E) methods provide an efficient alternative. In E-E framework, both the carrier and dispersed phases are treated as continua, with each phase described by its own set of conservation equations coupled through interphase momentum exchange terms [89, 90]. These exchange terms account for drag, pressure, and viscous interactions between the phases.

The most widely used E-E formulation is the Two-Fluid Model (TFM), in which separate conservation equations are solved for the fluid and particle phases. Since individual particles are not explicitly resolved, particle-scale interactions, collisions, and turbulence must be represented through models and closure relationships. Volume-filtered and volume-averaged formulations have also been developed to account for unresolved mesoscale structures and improve the modeling of interphase exchange terms [20–22].

An intermediate method between E-L and E-E methods is the Particle-in-Cell (PIC) method. Rather than tracking every particle individually, PIC represents groups of particles as computational parcels that are advanced in a Lagrangian reference frame while the carrier phase is solved on an Eulerian grid. Momentum exchange between the phases is computed using averaged parcel properties, reducing the computational cost compared to fully resolved E-L simulations while retaining information about particle trajectories [36].

Because neither TFM nor PIC resolves particle-scale flow structures, these methods are significantly less computationally expensive than particle-resolved

approaches and are therefore well suited for simulating industrial-scale systems such as fluidized beds, circulating fluidized reactors, risers, and pneumatic conveying systems [23–29].

1.1.2.5 REYNOLDS-AVERAGED NAVIER-STOKES SOLVERS Resolving the full range of turbulent motion in large-scale flows is computationally expensive.

Reynolds-Averaged Navier-Stokes (RANS) models overcome this limitation by solving the governing equations for the mean flow while modeling the effects of turbulent fluctuations through closure relationships. High-fidelity microscale and mesoscale simulations, such as E-L simulations, can provide time-averaged statistics for the development of these closure models. Because only the mean flow is solved, RANS simulations are significantly less computationally expensive than other frameworks, enabling simulations of large systems over long time scales. However, the accuracy of RANS predictions depends heavily on the turbulence closure model employed, and the framework cannot resolve instantaneous turbulent structures or transient mesoscale phenomena. The present work focuses on developing E-L-based closure relationships that can ultimately be incorporated into coarse-grained frameworks such as RANS.

1.1.3 PYROCLASTIC DENSITY CURRENTS

One society-critical example of a multiphase flow, and the motivation for this work, is pyroclastic density currents (PDCs)—the fast-moving, gravity-driven currents of volcanic particulate material that develop from the collapse of an eruptive column, a volcanic

dome, or unstable deposits perched on steep slopes [6]. PDCs are the most destructive volcanic processes due to their rapid propagation and high temperatures. PDCs are comprised of various volcanic materials (ash, fragmented magma, and rock) and hot volcanic gases. They are capable of overrunning large areas, destroying infrastructure, and causing severe impacts to ecosystems and human life [11, 14, 91].

Over the past decade, more than 650 fatalities have been attributed to PDCs, including events at Merapi (Indonesia, 2010), Ontake (Japan, 2014), Sinabung (Indonesia, 2014 and 2016), Fuego (Guatemala, 2018), Stromboli (Italy, 2019), and White Island (New Zealand, 2019) [6, 92–97]. Without geophysical monitoring, recorded fatalities from volcanic eruptions would be substantially higher. Pyroclastic density currents account for approximately one-third of all volcanic fatalities, exceeding those associated with most other volcanic processes, and nearly 100 million people worldwide currently live at risk from PDC hazards [6]. These factors underscore the critical importance of hazard-prediction modeling and effective risk-mitigation strategies.

In general, PDCs are comprised of three flow regions: An upper dilute buoyant region, a dilute to intermediate density region, and a concentrated basal underflow region (see Figure 1.5).

The dilute ash cloud behaves as a one-way coupled system, in which particles act largely as tracers and turbulence in the fluid dominates. In this region, particle-particle collisions are rare. Particle volume fraction is considered low ($\alpha_p \approx 10^{-3}$) and the flow contains many eddies ranging from the height of the flow down to small-scale turbulent

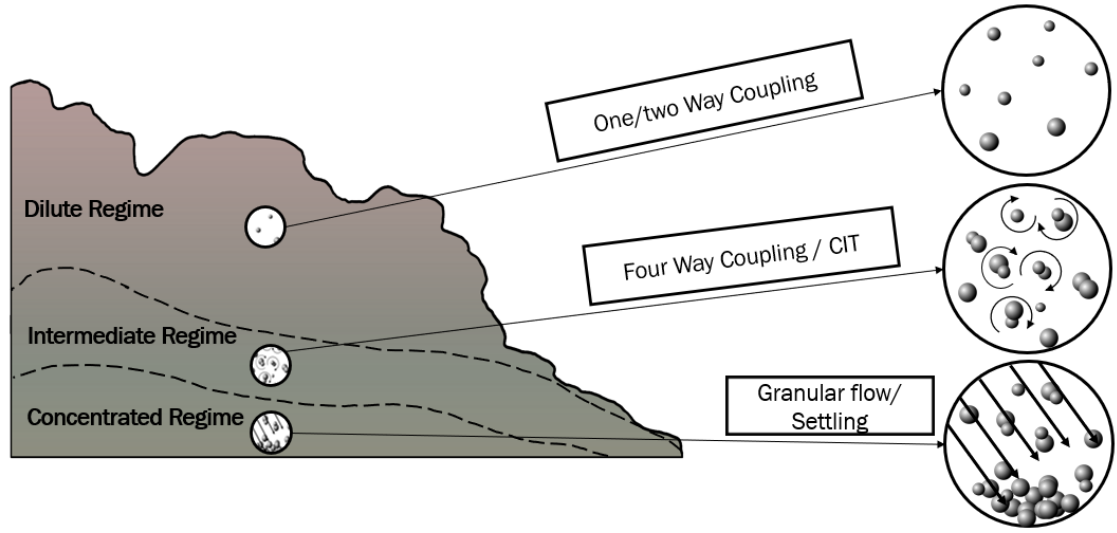


Figure 1.5: Anatomy of a pyroclastic density current showing the dilute ash cloud, the intermediate regime where settling particles form mesoscale clusters that generate cluster-induced turbulence (CIT), and the dense basal underflow characterized by granular flow behavior.

motion [6]. These turbulent eddies influence the flow in multiple ways. For example, they transfer energy from large swirling motions to smaller scales, where it is dissipated as heat; they affect how long particles stay suspended in the flow; and they modify how particles settle or are mixed within the current. The basal underflow, by contrast, is more concentrated ($\alpha_p > 0.30$), governed by bulk granular transport. The intermediate regime represents a critical transition zone where both particle-particle interactions and coupling between particles and fluid are significant. The intermediate region couples the turbulent ash cloud and basal underflow [6]. In this layer, clusters of particles spontaneously emerge, forming heterogeneous structures that generate and sustain turbulence in the surrounding fluid, as detailed previously as CIT [73, 98]. Clusters are more prominent in this area with particle volume fraction between $10^{-3} \leq \alpha_p \leq 0.30$. The formation of

clusters alters local fluid turbulence and particle behavior, making the intermediate regime critical for understanding PDC behavior.

PDCs have a wide range of particulate concentrations, making them difficult to quantify from direct observation. Field measurements, while essential for characterizing deposits and runout, typically yield post-eruption or time-averaged information and rarely capture transient flow behavior. This drawback has motivated the development of large-scale experiments [6, 11, 99–101] to capture this behavior.

The Pyroclastic Flow Eruption Large-scale Experiment (PELE) was among the first large-scale laboratory studies to achieve dynamic similarity with natural PDCs [12, 100]. Building on earlier work by Dellino [101], which focused primarily on vertical explosions, PELE omitted vertical eruption components, thereby enabling the generation of higher particle concentrations and volume fractions that are more representative of gravity-driven PDCs. This experimental configuration enabled the investigation of a broad range of particle transport processes and particle deposit behaviors associated with PDCs. PELE is an indoor experiment consisting of a device to eject natural PDC particles into the air, a horizontal runout section, pressure transducers, infrared sensors, and high-speed cameras to capture flow development along the horizontal channel. The same large-scale setup was later leveraged by Breard [11], who demonstrated that these experiments successfully reproduced key features of natural pyroclastic density currents, including dilute and concentrated flow regimes, flow stratification, turbulent entrainment, and realistic depositional patterns. Concentrated currents developed a dense basal underflow,

while dilute currents remained suspension-dominated. These results provide an important benchmark for validating numerical simulations of multiphase pyroclastic flows.

Numerical models and experiments play important roles in quantifying PDC behavior. The goal of models and experiments for PDCs is to quantify and characterize the behavior acting within these currents and relate them to observations of their deposits. Laboratory analog experiments can resolve more detailed flow features, but they are restricted by scale, material properties, and safety considerations, which limit their ability to replicate the full range of conditions present in natural events.

1.1.4 STATE OF THE ART MULTIPHASE FLOW AND PDC MODELS

The Mount St. Helens (1980), Montserrat (1995-1999), Tungurahua (2006), and Mt. Tongariro (2012) eruptions [14, 102] provide detailed information on the multiphase nature of PDCs, including ash runout distance, particle makeup, and overall deposit thickness that are used as inputs to state-of-the-art PDC simulations and models. Within the last few decades, numerous mathematical models have been created to predict the behavior of PDCs. These models generally fall under three categories: (1) dilute box model approaches, (2) depth-averaged concentrated flow models, and (3) 3D multiphase models. Environmental and surface conditions strongly influence eruption behavior and hazards. Dry and clear conditions produce PDCs dominated by gravity-driven turbulent flow where strong air entrainment controls particulate settling, and particles can remobilize after settling has occurred. When rain is present [103, 104], there is increased

near-surface moisture, potentially enhancing short-term mobility but accelerating rapid collapse. In the presence of snow/ice [105–108], thermal exchange with snow/ice generates steam, enhancing local turbulence. In glacial and groundwater-rich systems [109, 110], enhanced fine-particle production increases bulk density and promotes radial spreading. Strong wind conditions [111, 112] tilt eruption columns and shift collapse zones laterally, which can induce asymmetric PDC placement. These conditions affect PDC behavior and, in some computational methods, must be modeled for accurate results [11, 113].

1.1.4.1 ONE-DIMENSIONAL VOLCANIC MODELS One-dimensional volcanic models are among the simplest frameworks used to investigate volcanic plumes and PDCs. By reducing the governing equations to a single spatial dimension, these models provide computationally efficient tools for studying large-scale flow behavior and rapidly exploring parameter space. Although the specific formulations differ between eruption columns and gravity-driven currents, both approaches rely on bulk-averaged conservation equations and modeled representations of unresolved physical processes.

For eruption columns, one-dimensional plume models originate from buoyant plume theory and describe plume evolution using conservation equations for mass, momentum, and energy along the plume centerline [14, 15, 114–122]. Turbulent mixing is not resolved directly and is instead represented through entrainment relationships that account for the addition of ambient air into the plume. In this framework, plume

properties are represented using bulk averages. This simplification allows rapid exploration of eruption parameters while retaining the important processes governing plume development, including buoyancy, entrainment, particle settling, and atmospheric interactions. As a result, one-dimensional plume models remain widely used for eruption forecasting and hazard assessment.

Because volcanic plumes are generally dilute, particle-particle interactions are often assumed to have a negligible influence on the bulk plume behavior. Modern one-dimensional plume models incorporate additional physics such as particle fallout, multiple particle sizes, atmospheric conditions, phase changes, and wind effects.

Early and widely used formulations, such as Puffin [14, 123], account for the effects of wind on plume development. Puffin incorporates particle grain size as an input parameter and includes particle settling, particle entrainment, and stratification effects [124]. Further details on this model can be found in Pouget [14]. Other models, including those of Degruyter [114], PlumeMoM [120, 125], Devenish [121, 126], Plumeria [127–129], FPlume [118, 130], PlumeRise [131, 132], Paris Plume Model (PPM) [133, 134], and Dusty-1D [135], extend the governing equations to include atmospheric effects such as humidity, phase changes, and environmental interactions.

PlumeMoM [120] introduces a moment-based description of particle size distributions while accounting for polydispersity and particle settling. FPlume [118] provides one of the most comprehensive one-dimensional plume formulations, including

wind effects [123], particle settling and re-entrainment, ambient moisture, water phase changes, and wet aggregation, and is commonly used for hazard prediction.

In addition to eruption-column models, one-dimensional approaches have also been developed for PDCs. These models are commonly formulated as box models or depth-averaged gravity-current models, in which the flow is represented using bulk-averaged quantities such as flow depth, velocity, and density. Unlike plume models, which primarily describe vertical transport, one-dimensional PDC models are used to investigate current mobility, runout distance, deposition, and interactions with topography. Vertical variations within the flow are neglected or represented through modeled relationships.

In the simplest one-dimensional steady-state form (based on [136, 137]), the conservation equations for mass and momentum reduce to

$$\frac{d}{dx}(hu) = 0 \quad (1.9)$$

$$\frac{d}{dx} \left(hu^2 + \frac{1}{2}gh^2 \right) = -gh \frac{dB}{dx}, \quad (1.10)$$

where x is the horizontal coordinate along the flow direction, $u(x)$ is the depth-averaged flow velocity, $h(x)$ is the flow thickness, $B(x)$ is the bed (or topographic) elevation, and g is the acceleration due to gravity.

A representative schematic of the one-dimensional PDC framework is shown in Figure 1.6. In the figure, the horizontal and vertical coordinates are denoted by x and z ,

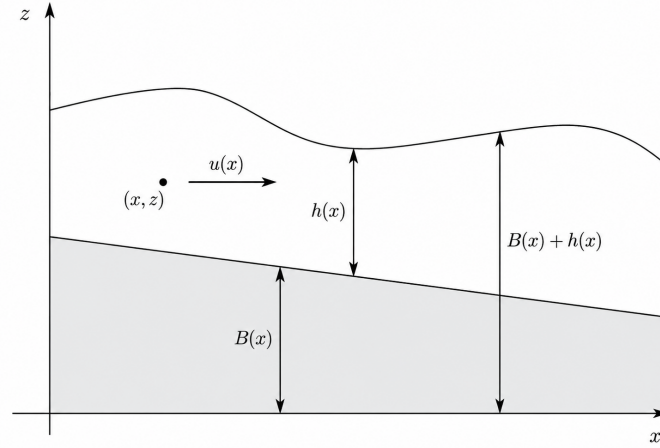


Figure 1.6: Schematic representation of a one-dimensional flow model illustrating the free-surface elevation, $h(x)$, above a spatially varying bed topography, $B(x)$. The velocity components $u(x)$ and total flow depth, $B(x) + h(x)$, are shown within the x - z plane. Adapted from [138].

respectively. The free-surface elevation is given by $B(x) + h(x)$, illustrating the relationship between the underlying topography and the overlying flow thickness.

Overall, one-dimensional volcanic models represent eruption columns and PDCs using bulk-averaged conservation equations and parameterized representations of unresolved physical processes. While modern formulations can incorporate a wide range of physical processes, particle-scale interactions, particle clustering, CIT, and granular-flow behavior are not captured explicitly and must instead be represented through empirical or semi-empirical models.

1.1.4.2 TWO-DIMENSIONAL VOLCANIC MODELS Depth-averaged

two-dimensional models are commonly used when the characteristic flow depth is much smaller than the horizontal length scales of the flow. Under this assumption, the governing

equations are integrated over the flow thickness, reducing a three-dimensional problem to two spatial dimensions. This approach significantly reduces computational cost while retaining the important horizontal flow dynamics. Depth-averaged models represent the flow using bulk-averaged quantities, while particle transport and multiphase interactions can be incorporated through additional transport equations and closure relationships when required [139, 140].

For simplicity, the incompressible, inviscid, and steady-state depth-averaged conservation equations are presented here. The conservation of mass is given by

$$\frac{\partial(hu)}{\partial x} + \frac{\partial(hv)}{\partial y} = 0, \quad (1.11)$$

The corresponding momentum equations in the x and y directions are

$$\frac{\partial(hu^2)}{\partial x} + \frac{\partial(huv)}{\partial y} + gh \frac{\partial(h+B)}{\partial x} = 0, \quad (1.12)$$

$$\frac{\partial(huv)}{\partial x} + \frac{\partial(hv^2)}{\partial y} + gh \frac{\partial(h+B)}{\partial y} = 0. \quad (1.13)$$

where $h(x, y)$ is the flow thickness, $B(x, y)$ is the bed elevation, and u and v are the depth-averaged velocity components in the x and y directions, respectively.

A representative diagram for two-dimensional depth-averaged models is shown in Figure 1.7. In Eqs. (1.12) and (1.13), the final term accounts for the gravitational force associated with variations in the elevation. The equations presented here do not include

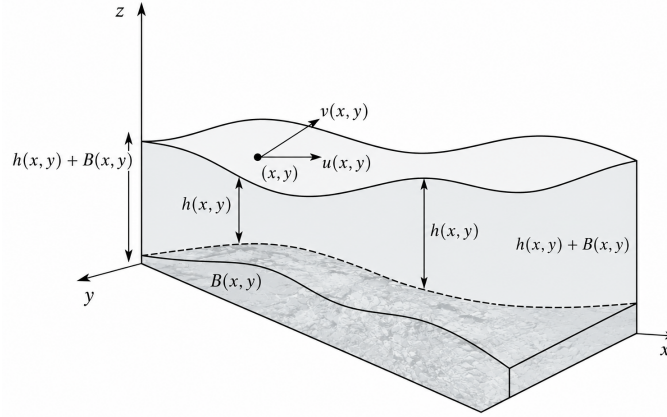


Figure 1.7: Schematic representation of a two-dimensional depth-averaged flow model illustrating the free-surface elevation, $h(x, y)$, above a spatially varying bed topography, $B(x, y)$. The depth-averaged velocity components, (u, v) , and total flow depth, $B(x, y) + h(x, y)$, are also shown.

additional physical processes such as particle deposition, entrainment of ambient air or water vapor, basal friction, interphase drag, thermal effects, or energy transport.

Because the governing equations are averaged over the flow depth, vertical flow structure is not resolved directly. As a result, depth-averaged models cannot capture vertical stratification and do not resolve particle-scale interactions or mesoscale structures such as particle clustering. These effects must instead be represented through closure relationships. Despite these limitations, depth-averaged equations have been applied successfully to a wide range of environmental flows, including storms [141], tsunamis (with a sedimentary seabed) [142], oceanic flows [143, 144], and avalanches [145–148]. In volcanology, depth-averaged models have been used to describe ash cloud spreading [149, 150], lahar formation (a rapidly flowing mixture of water, volcanic ash, rock

fragments, and sediment that moves downslope under the influence of gravity) and transport [151], lava flows [152–154], and PDCs [155–161].

TITAN2D [16] is a depth-averaged numerical model used to simulate gravity-driven granular flows over complex terrain. The flow is treated as an incompressible granular material, and the model solves simplified conservation equations for mass and momentum using friction terms to represent interactions within the flow and at the terrain. The model provides estimates of flow thickness, velocity, and runout distance.

IMEX-SfloW2D [138, 162] is a depth-averaged framework developed for geophysical flows. Unlike simpler depth-averaged formulations, IMEX-SfloW2D includes transport equations for multiple particle sizes, sedimentation and entrainment source terms, and a temperature/energy model. Particle settling is represented through closure relationships that depend on local flow conditions and particle properties [89]. A complete mathematical description of the framework is provided by de’Michieli Vitturi [138]. The studies presented in this dissertation leverage equations and data from IMEX-SfloW2D as a point of comparison.

Overall, depth-averaged two-dimensional models provide a computationally efficient framework for simulating large-scale volcanic flows over complex terrain. While modern formulations can incorporate particle transport, sedimentation, entrainment, and thermal effects, the depth-averaging procedure removes vertical flow structure and does not resolve particle-scale interactions. Consequently, mesoscale phenomena such as

particle clustering and cluster-induced turbulence must be represented through closure relationships.

1.1.4.3 THREE-DIMENSIONAL VOLCANIC MODELS Three-dimensional models of PDCs solve the time-dependent conservation equations for mass, momentum, and energy in all three spatial dimensions based on the Navier-Stokes equations [6, 19, 152, 163, 164]. Depending on the computational framework, these equations may be solved directly or combined with turbulence models through LES or RANS formulations. Unlike one-dimensional and depth-averaged two-dimensional approaches, three-dimensional models retain the complete spatial structure of the flow and can represent complex interactions with topography, atmospheric conditions, and multiphase transport processes. Depending on the modeling framework, the fluid-particle mixture may be treated either as a single bulk continuum or as multiple interacting phases. In continuum approaches, the particulate phase is incorporated through bulk mixture properties, whereas multiphase formulations solve separate conservation equations for the fluid and particulate phases and couple them through interphase momentum and heat exchange terms.

Commonly used three-dimensional volcanic flow models include Active Tracer High Resolution Atmospheric Model (ATHAM) [165], SK-3D [166, 167], and PDAC [168–170]. These models have been used to investigate volcanic plumes, PDCs, and ash transport under a wide range of eruption and atmospheric conditions. By resolving the full

three-dimensional flow field, they provide significantly greater fidelity than reduced-order one-dimensional and depth-averaged models.

Ash Equilibrium-Eulerian (ASHEE) is a three-dimensional multiphase framework used to simulate turbulent volcanic plumes and PDCs [122, 169]. The model treats both the fluid and particulate phases as separate continua and is based on turbulent dispersed multiphase flow theory [171]. Because the framework assumes dilute suspensions, particle-particle collisions are neglected, and particle transport is governed primarily by fluid-particle interactions. These assumptions are generally appropriate for dilute volcanic plumes and ash clouds, where collisions between particles are typically negligible.

Volcanic Ash Transport and Dispersion (VATD) models [164] are another important class of three-dimensional volcanic flow models. These frameworks are used to predict the transport, dispersion, and deposition of volcanic ash following an eruption. Atmospheric conditions, turbulence, and particle settling are incorporated to estimate ash concentrations, deposit thicknesses, and ash arrival times in downwind regions. Because different particle sizes settle at different rates, these models often include multiple particle sizes to capture the effects of polydispersity. VATD models are widely used for hazard assessment, aviation safety, and eruption response planning.

These models have been used to quantify the important physics of PDCs that are inaccessible by large-scale experimentation and to develop improved reduced-order forecasting models. A large majority of existing models are used to describe bulk behavior and not necessarily a specific regime within a volcano or PDC. Although the

intermediate regime constitutes only a small portion of a volcanic eruption, it plays an important role in predicting how these flows behave. Accurately predicting the dynamics of these flows remains extremely difficult due to the complex interactions between phases and the breadth of temporal and spatial scales over which these processes occur. These challenges have historically hindered the development of predictive models. Of particular interest is particle settling time, which is altered by multiphase behavior. Understanding the physics of settling could aid predictions for ash runout length.

1.2 OBJECTIVES OF THIS WORK

As discussed in the previous sections, the wide range of spatial scales present in these flows, from particle-fluid interactions at the grain scale to kilometer-scale hazardous currents, cannot be simultaneously resolved within a single computational framework while remaining computationally feasible. Consequently, large-scale multiphase flow models rely on closure relationships to represent unresolved particle-fluid and particle-particle interactions. The predictive capability of these models therefore depends on the accuracy with which the closures represent the underlying micro- and mesoscale physics [43, 81, 89].

Many predictive models also rely on *a priori* predictors, quantities that can be evaluated from known flow properties to estimate behavior. Examples include Stokes settling velocity and particle Reynolds number. While these predictors have proven useful for simplified systems, they are typically derived from isolated particles, monodisperse

suspensions, or homogeneous flows. As a result, they do not adequately describe the collective particle dynamics associated with polydispersity, particle clustering, and CIT [43, 44, 172].

Particle settling provides one example of these limitations. Classical settling assumptions, such as Stokes' law, assume isolated particles settling in a quiescent fluid and therefore neglect particle-particle interactions, turbulence, and clustering [173]. Numerous studies have extended Stokes' formulation by incorporating particle Reynolds number, drag correlations, and particle shape effects [174–185]. Although these formulations improve predictions over a wider range of flow conditions, they remain fundamentally single-particle descriptions and cannot capture the effects of particle clustering or CIT.

Similar limitations exist in many closure relationships used by coarse-grained multiphase flow models. Consequently, current volcanological models cannot fully capture the effects of particle clustering on transport and deposition, limiting their predictive capability [20, 44–47].

The primary objective of this dissertation is to develop new *a priori* predictors and closure relationships for polydisperse particle-laden flows using high-fidelity E-L simulations. By resolving particle-fluid interactions and the emergence of particle clusters, these simulations provide the statistical data needed to identify physically meaningful predictors and characterize unresolved multiphase processes. The resulting closure relationships are intended for incorporation into coarse-grained multiphase flow

solvers, improving the predictive capability of large-scale PDC simulations while remaining broadly applicable to other polydisperse multiphase flow systems.

1.3 DISSERTATION OUTLINE

Chapter 2 describes the computational framework used throughout this dissertation, including the governing equations, numerical methods, and simulation setup in the high-fidelity E-L simulations. Chapter 3 presents a detailed investigation of particle clustering and settling behavior in polydisperse particle-laden flows, leading to the development of new *a priori* predictors and closure relationships. Chapter 4 investigates the effects of computational domain size on steady-state statistics and develops scaling relationships that describe how key flow statistics vary with domain size. Chapter 5 investigates the effects of spatial filtering on fluid-particle statistics and develops closure relationships that account for unresolved sub-filter-scale behavior. Finally, Chapter 6 summarizes the major findings of this dissertation, discusses the broader implications of the proposed modeling framework, and provides recommendations for future research.

CHAPTER 2

SIMULATION FRAMEWORK AND MATHEMATICAL DESCRIPTION

The following subsections detail the mesoscale and macroscale equations needed to describe the motion of spherical, collisional, solid particles inside an incompressible fluid, beginning with a discussion on the employed computational methodology in this study, followed by the mesoscale descriptions of the fluid and particle phases and the equations needed to describe the coupling between phases. Lastly, important time-averaged quantities of interest are presented.

2.0.1 SIMULATION FRAMEWORK: NGA

NGA is a computational fluid dynamics (CFD) code developed for high-fidelity simulations of particle-laden turbulent flows [73, 81]. The solver employs a fully conservative, finite-volume formulation to solve the low-Mach-number Navier-Stokes equations on an Eulerian mesh while the dispersed phase is represented by individual Lagrangian particles. Spatial discretization is second-order accurate for both the convective and viscous terms. Time advancement of the fluid phase is performed using a second-order semi-implicit Crank-Nicolson scheme based on the method of Pierce and Moin [186]. The numerical algorithm follows a fractional-step approach, employing both spatial and temporal staggering of the velocity, pressure, and density fields to satisfy mass

conservation. Particle volume fraction is stored at cell centers, consistent with the density field.

In the present work, particles are modeled as rigid, perfectly spherical bodies, neglecting irregular particle shape, surface roughness, and deformation. This assumption simplifies the particle dynamics while preserving the dominant mechanisms governing particle settling, clustering, and particle-fluid interactions. Each particle is characterized by its position, volume, and velocity, denoted by $\mathbf{x}_p^{(i)}$, $V_p^{(i)}$, and $\mathbf{u}_p^{(i)}$, respectively. Initially, particles are randomly distributed throughout the computational domain while the carrier fluid is quiescent.

A schematic of the computational domain is shown in Figure 2.1. The domain dimensions are scaled using the characteristic cluster length, $\mathcal{L} = \tau_p^2 g$, which provides an estimate of the characteristic cluster size. The computational domain is selected to be several characteristic cluster lengths in each direction to ensure statistically representative cluster formation. Consequently, the domain dimensions are given by $L_x \times L_y \times L_z$. Gravity is prescribed in the negative x -direction, with its magnitude adjusted to satisfy the desired characteristic domain length. The computational mesh is uniform with a grid spacing of $\Delta x = 1.75 d_{p,\min}$. The number of cells in each direction is computed from the corresponding domain length divided by the grid spacing. The computational domain is triply periodic with constant temperature, fluid density, particle density, and fluid viscosity.

Prior to each fluid solver time step, an Adams-Bashforth predictor estimates the intermediate fluid velocity experienced by the particles. This predictor provides

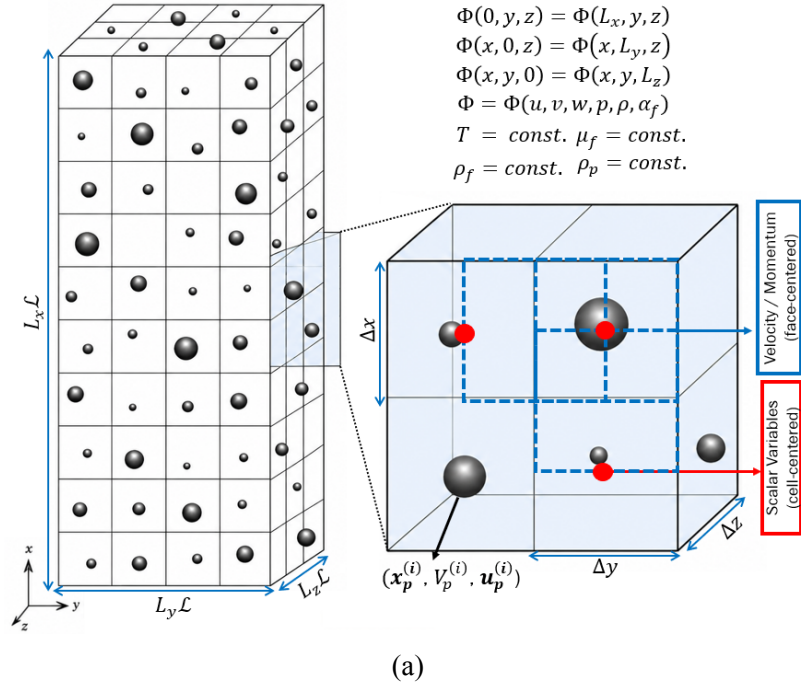


Figure 2.1: Representative computational domain used in NGA. The left panel illustrates the triply periodic computational domain populated with discrete Lagrangian particles. The right panel shows the staggered Eulerian mesh, where scalar quantities (pressure, density, and volume fraction) are stored at cell centers, while momentum and velocity components are stored at cell faces. Particle properties, including position, volume, and velocity, are tracked independently of the Eulerian mesh and coupled to the fluid through interpolation and filtering. Constant fluid and particle properties are assumed throughout the simulations.

second-order temporal accuracy for the particle-fluid coupling [81]. The particle equations of motion consist of nine coupled ordinary differential equations per particle and are integrated using a second-order Runge-Kutta scheme. For cases where the particle response time becomes smaller than the fluid solver time step, particle sub-stepping is employed to maintain numerical stability [81].

Particle collisions are modeled using the soft-sphere collision model of Cundall and Strack [187], in which particles are treated as inelastic and frictional. Collision detection is performed by searching the $3 \times 3 \times 3$ stencil of neighboring cells surrounding

each particle. Interphase momentum exchange and particle volume fraction are subsequently projected onto the Eulerian mesh through a filtering operation, providing two-way coupling between the particle and fluid phases. Details of the filtering methodology are presented in Section 2.0.1.3. The fluid equations are then advanced using the Crank-Nicolson scheme to complete the time step.

The solver is parallelized using the Message Passing Interface (MPI). Particles are distributed among processors according to the underlying Eulerian domain decomposition. As particles migrate across processor boundaries, neighboring processors exchange particle information through ghost cells. Particles entering the ghost region of an adjacent processor are communicated to that processor and subsequently removed from the originating processor to maintain data consistency. A representative schematic of the interprocessor communication procedure is shown in Figure 2.2 [81].

Following an initial transient period, the flow reaches a statistically stationary state. Statistical stationarity is assessed by monitoring the mean particle settling velocity together with the variance of the particle volume fraction until both quantities fluctuate about constant mean values.

2.0.1.1 FLUID-PHASE DESCRIPTION To account for the presence of particles in the fluid phase without explicitly resolving the flow surrounding every individual particle, a volume filter is applied to the incompressible Navier-Stokes equations [188]. Volume filtering is a spatial averaging procedure in which the governing equations are averaged

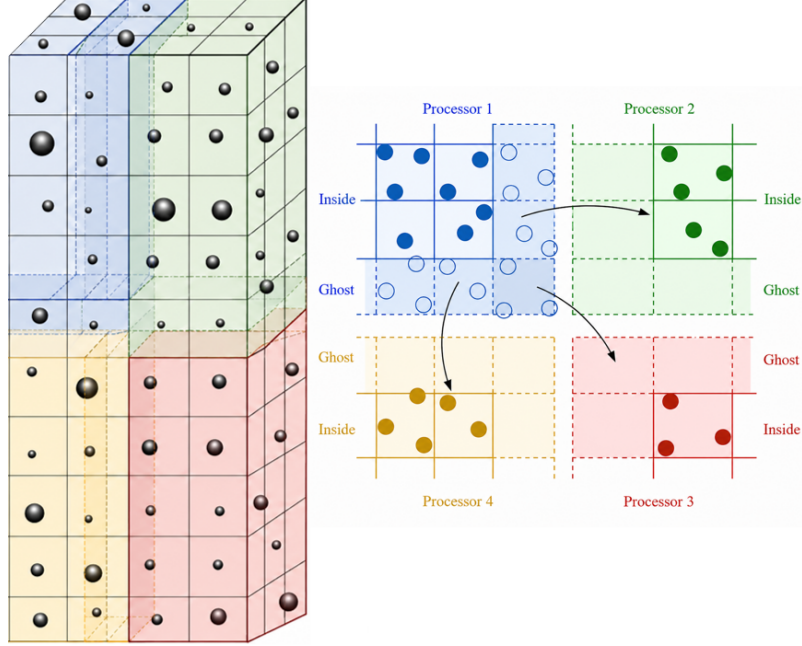


Figure 2.2: Representative schematic detailing the procedure for sharing particle data between processors adapted from [81]. Here the solver is parallelized using the Message Passing Interface (MPI). Interprocessor communication is performed through ghost cells, where particles crossing processor boundaries are transferred to neighboring processors and removed from the originating processor to maintain data consistency. Image generated using AI-assisted visualization tools.

over a finite control volume that is large compared to the particle diameter but small relative to the overall flow. This operation replaces pointwise microscale variables, such as the fluid velocity and pressure, with smooth, locally averaged fields that describe the bulk fluid behavior within the filter volume. As a result, particle-scale flow structures, including boundary layers and wakes, are no longer resolved explicitly. The primary advantage of this approach is that it greatly reduces the computational cost. However, because particle-scale information is removed during the filtering process, sub-filter phenomena such as interphase drag and particle–particle collision forces must be modeled rather than computed directly [189]. Throughout this section, vectors and tensors are

denoted using boldface notation. The resulting volume-filtered governing equations are,

$$\frac{\partial (\alpha_f \rho_f)}{\partial t} + \nabla \cdot (\alpha_f \rho_f \mathbf{u}_f) = 0 \quad (2.1)$$

$$\frac{\partial (\alpha_f \rho_f \mathbf{u}_f)}{\partial t} + \nabla \cdot (\alpha_f \rho_f \mathbf{u}_f \otimes \mathbf{u}_f) = \nabla \cdot \boldsymbol{\tau}_f + \alpha_f \rho_f \mathbf{g} + \mathcal{F} + \mathbf{F}_{\text{mfr}}, \quad (2.2)$$

where α_f is the fluid volume fraction, $\mathbf{u}_f$ is the fluid velocity vector, and ∇ is the vector differential operator. The symbol $\otimes$ denotes the dyadic (outer) product of two vectors. The fluid-phase viscous stress tensor is represented by $\boldsymbol{\tau}_f$, $\mathbf{g}$ is the gravitational acceleration vector, $\mathcal{F}$ is the interphase momentum exchange force accounting for two-way coupling between the fluid and particle phases, and $\mathbf{F}_{\text{mfr}}$ is a momentum source term used to maintain a constant mass flow rate and achieve a statistically stationary state. The fluid-phase viscous-stress tensor is defined as

$$\boldsymbol{\tau}_f = -p\mathbb{I} + \rho_f(\nu_f + \nu_f^*)[\nabla \mathbf{u}_f + (\nabla \mathbf{u}_f)^T - \frac{2}{3}\nabla \cdot \mathbf{u}_f\mathbb{I}], \quad (2.3)$$

where p is the fluid pressure, $\mathbb{I}$ is the second-order identity tensor, ν_f^* is the turbulent (or sub-filter-scale) eddy viscosity (an unclosed term resulting from volume filtering the microscopic fluid stress tensor), $\nabla \mathbf{u}_f$ is the fluid velocity gradient tensor, $(\nabla \mathbf{u}_f)^T$ is its transpose, and $\nabla \cdot \mathbf{u}_f$ is the velocity divergence. The term in brackets accounts for viscous deformation of the fluid. The viscous stress tensor is modeled using the Boussinesq eddy-viscosity assumption [54], where the effective viscosity is the sum of

the molecular viscosity and the subgrid-scale eddy viscosity given as

$$\nu_{\text{eff}} = \nu_f + \nu_f^*. \quad (2.4)$$

These unresolved stresses account for the additional dissipation associated with fluid velocity fluctuations generated at the particle scale. A variety of theoretical and semi-empirical models for the effective viscosity have been proposed [190–192]. These models are commonly expressed as functions of local particle-phase volume fraction, particle Reynolds number, and mass loading. The closure of terms involving ν_f^* does not notably influence the flow physics and is small enough to be neglected, as shown in a corresponding monodisperse study of Capecelatro et al. [73].

2.0.1.2 PARTICLE-PHASE DESCRIPTION The dispersed phase is solved using Lagrangian mechanics. The position and velocity of the i -th particle are calculated according to Newton’s second law

$$\frac{d\mathbf{x}_p^{(i)}}{dt} = \mathbf{u}_p^{(i)} \quad (2.5)$$

$$m_p^{(i)} \frac{d\mathbf{u}_p^{(i)}}{dt} = \mathbf{F}_{\text{inter}} + \mathbf{F}_{\text{col}} + m_p^{(i)} \mathbf{g}, \quad (2.6)$$

where $\mathbf{x}_p^{(i)}$ is the center position of particle i , $\mathbf{u}_p^{(i)}$ is its velocity at time t , and $\mathbf{g} = (-g, 0, 0)^T$ is the gravitational acceleration vector. Particle mass is defined as $m_p = \frac{\pi \rho_p d_p^3}{6}$. The force due to inter-particle collisions, $\mathbf{F}_{\text{col}}$, is modeled using the

soft-sphere collision model proposed by Cundall and Strack [187]. Particles are treated as inelastic and frictional with a coefficient of restitution of 0.85 and a coefficient of friction of 0.10. These values represent moderately inelastic collisions that are characteristic of hard granular materials and have been widely adopted in particle-laden flow simulations. Furthermore, the same collision parameters were employed in the corresponding monodisperse study of Capecelatro et al. [73], allowing direct comparison between the monodisperse and polydisperse simulations while maintaining consistency in the collision model. As shown in Eq. (2.6), particles are subject to three forces: the force due to interphase momentum exchange, $\mathbf{F}_{\text{inter}}$, the force due to inter-particle collisions, $\mathbf{F}_{\text{col}}$, and the body force. Here, the interphase momentum exchange force acting on particle i is given by

$$\mathbf{F}_{\text{inter}}^{(i)} = V_p^{(i)} \nabla \cdot \boldsymbol{\tau}_f[\mathbf{x}_p^{(i)}] + \frac{m_p^{(i)} \alpha_f [\mathbf{x}_p^{(i)}] F_d(\alpha_f, \text{Re}_p^{(i)})}{\tau_p^{(i)}} (\mathbf{u}_f[\mathbf{x}_p^{(i)}] - \mathbf{u}_p^{(i)}), \quad (2.7)$$

where $\tau_p^{(i)}$ is the particle response time, $\mathbf{u}_f[\mathbf{x}_p^{(i)}]$ is the fluid velocity interpolated to the particle location, $\mathbf{u}_p^{(i)}$ is the particle velocity, and F_d is the non-dimensional drag correction proposed by Tenneti et al. [44], which accounts for the effects of local solids concentration and particle Reynolds number.

The drag correction is given by

$$F_d(\alpha_f, \text{Re}_p) = \frac{1 + 0.15 \text{Re}_p^{0.687}}{\alpha_f^2} + \alpha_f F_1(\alpha_f) + \alpha_f F_2(\alpha_f, \text{Re}_p), \quad (2.8)$$

where the local particle Reynolds number is defined as

$$\text{Re}_p^{(i)} = \frac{\alpha_f[\mathbf{x}_p^{(i)}] \left| \mathbf{u}_f[\mathbf{x}_p^{(i)}] - \mathbf{u}_p^{(i)} \right| d_p}{\nu_f} \quad (2.9)$$

with d_p denoting the particle diameter and ν_f the fluid kinematic viscosity. The fluid-phase volume fraction is related to the particle volume fraction through $\alpha_f = 1 - \alpha_p$.

The empirical correction functions are given by

$$F_1(\alpha_f) = \frac{5.81\alpha_p}{\alpha_f^3} + \frac{0.48\alpha_p^{1/3}}{\alpha_f^4} \quad (2.10)$$

$$F_2(\alpha_f, \text{Re}_p) = \alpha_p^3 \text{Re}_p \left(0.95 + \frac{0.61\alpha_p^3}{\alpha_f^2} \right), \quad (2.11)$$

where F_1 accounts for the influence of local solids concentration on the drag force, while F_2 provides an additional correction for finite particle Reynolds number effects.

The drag correction proposed by Tenneti et al. [44] is adopted because it accounts for the influence of both local solids volume fraction and particle Reynolds number on the interphase drag force. Unlike isolated-particle drag correlations, this model was developed using particle-resolved direct numerical simulations (PR-DNS), enabling it to capture interactions between neighboring particles in moderately dense suspensions. These effects are particularly important for the particle volume fractions considered in this work, where local clustering modifies the drag experienced by individual particles. Furthermore, this drag model was employed in the corresponding monodisperse study of Capecelatro et al.

[73], allowing direct comparison between the monodisperse and polydisperse simulations while ensuring consistency in the underlying interphase force model.

2.0.1.3 INTERPHASE MOMENTUM EXCHANGE Coupling between the fluid and particle phases occurs through the particle volume fraction and the interphase momentum exchange. Because the particles are represented as discrete Lagrangian points while the fluid is solved on an Eulerian mesh, particle information must be transferred between the two numerical descriptions. Directly assigning particle properties to the nearest grid cell produces discontinuous fields and large cell-to-cell variations that can introduce numerical noise and degrade solution accuracy. To obtain smooth, continuous Eulerian fields, a two-step filtering procedure originally developed by Capecelatro et al. [73, 81] is employed. The same filtering methodology is adopted in the present work to maintain consistency with the corresponding monodisperse study, thereby enabling direct comparison between the monodisperse and polydisperse simulations.

Particle-localized quantities are first deposited onto the surrounding Eulerian mesh using tri-linear interpolation. The deposited fields are subsequently smoothed by solving an implicit Laplacian diffusion equation along each coordinate direction using an alternating-direction implicit (ADI) scheme. This procedure distributes the influence of each particle over a finite region of the computational mesh, producing smooth particle volume fraction and momentum exchange fields while preserving the total particle mass and momentum.

The amount of smoothing is controlled by the filter full width at half maximum (FWHM), denoted by δ_f . This parameter defines the effective spatial extent over which each particle influences the surrounding Eulerian cells and is related to the standard deviation, σ , by

$$\sigma = \frac{\delta_f}{2\sqrt{2\ln 2}} \quad \Longleftrightarrow \quad \delta_f = 2\sqrt{2\ln 2} \sigma. \quad (2.12)$$

Larger values of δ_f distribute particle information over a wider region of the computational mesh, resulting in smoother Eulerian fields. Conversely, smaller values preserve more localized particle information but may introduce larger spatial gradients and numerical noise.

Following the filtering operation, the particle-phase volume fraction is defined as

$$\alpha_f = 1 - \sum_{i=1}^{N_p} H(|\mathbf{x} - \mathbf{x}_p^{(i)}|) V_p^{(i)}, \quad (2.13)$$

where N_p is the total number of particles and H is the smoothing kernel generated by the implicit Laplacian filter.

Similarly, the filtered interphase momentum exchange is given by

$$\mathcal{F} = - \sum_{i=1}^{N_p} H(|\mathbf{x} - \mathbf{x}_p^{(i)}|) \mathbf{F}_{\text{inter}}^{(i)}. \quad (2.14)$$

These filtered quantities provide the coupling between the Lagrangian particle solver and the Eulerian fluid solver. A representative illustration of the filtering procedure detailed herein is shown in Figure 2.3.

2.0.1.4 PHASE-AVERAGED QUANTITIES OF INTEREST For high-inertia multiphase flows, where both the continuous and dispersed phases experience high-frequency velocity fluctuations, it is often necessary to average these fluctuations to focus on time-averaged quantities of interest. Particle-laden flows have two ways in which velocity fluctuations can occur: particle-particle collisions and particle-fluid wake instabilities, and as such, common Reynolds stress closures (used in single-phase flows) can not be leveraged. Particles tend to deviate from fluid path-lines and, as such, can become uncorrelated.

A phase-averaging (PA) method, derived by taking the Reynolds average of the volume-filtered quantities, was leveraged. Phase averaging, which is analogous to Favré averaging for variable-density flows, are denoted by $\langle(\cdot)\rangle_p = \langle\alpha_p(\cdot)\rangle/\langle\alpha_p\rangle$ and $\langle(\cdot)\rangle_f = \langle\alpha_f(\cdot)\rangle/\langle\alpha_f\rangle$. Phase averages are denoted with angled brackets and a subscript f or p to indicate the phase with respect to which the average has been taken. Angled brackets without a subscript indicate a standard Reynolds average, which consists of an average of the overall spatial dimension in this work. Since this work is triply periodic, a Reynolds average of an Eulerian quantity represents a volume average. Lagrangian quantities are calculated as ensemble averages. Due to the stationarity in time, both Eulerian and Lagrangian quantities are also Reynolds averaged over time in an ensemble

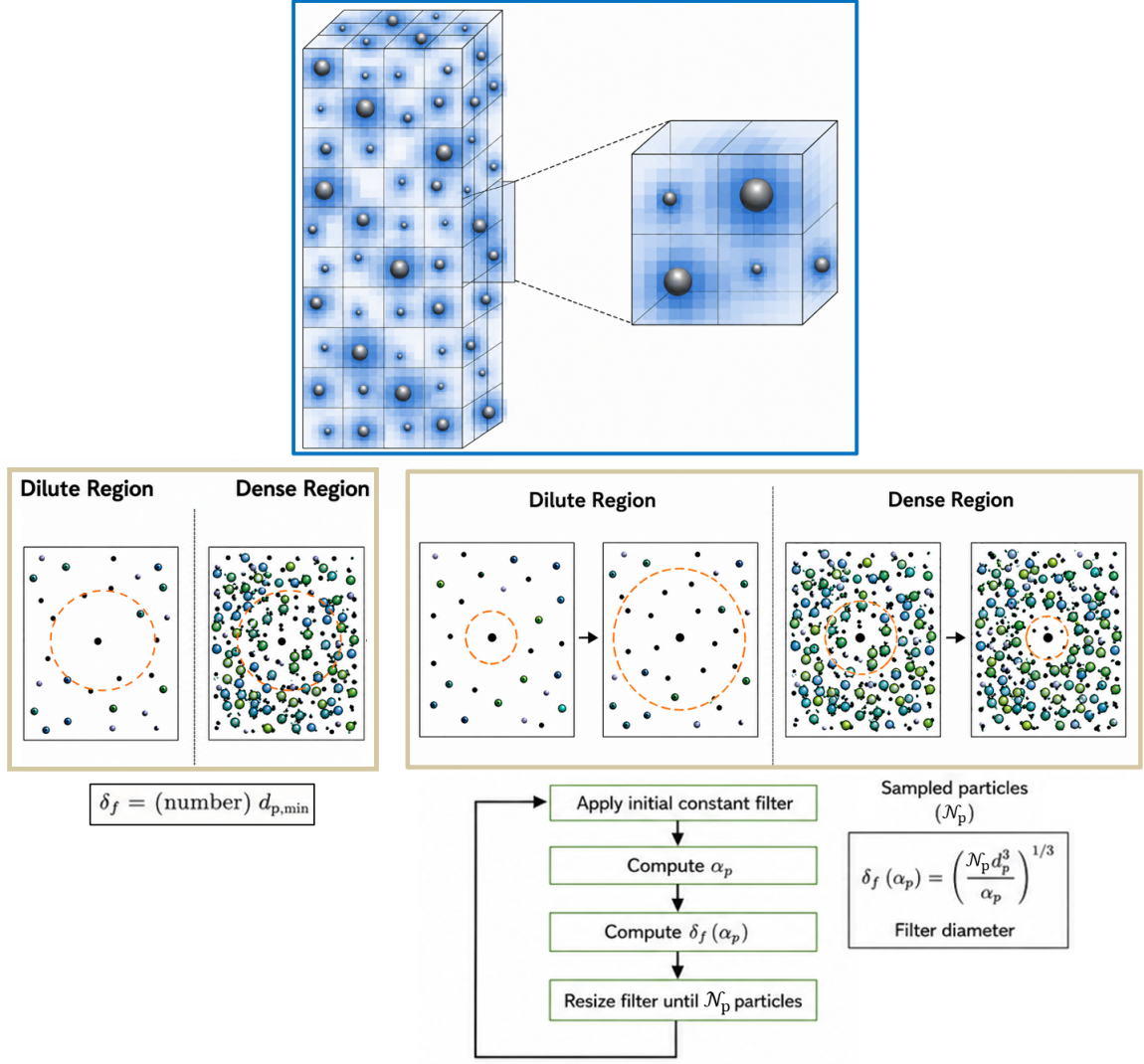


Figure 2.3: Illustration of the adaptive filtering procedure used to transfer Lagrangian particle information onto the Eulerian mesh. Top: Representation of particle filtering within the simulated Eulerian domain. Discrete particle properties are distributed over neighboring grid cells through tri-linear interpolation, producing continuous particle fields. The enlarged inset demonstrates how the influence of each particle is distributed over multiple Eulerian cells rather than being assigned to a single grid location. Bottom: Comparison of fixed and adaptive filtering approaches in dilute and dense particle regions. In each schematic, the solid black particle denotes the sampled particle, while the orange dashed circle represents a two-dimensional projection of the three-dimensional filtering volume. For a fixed filter, the filtering volume remains constant regardless of the local particle concentration, resulting in fewer sampled particles in dilute regions and more sampled particles in dense regions. In the adaptive filtering approach, the filter diameter is adjusted according to the local particle volume fraction to maintain a constant number of sampled particles, $\mathcal{N}_p$. Image generated using AI-assisted visualization tools.

sense, i.e.,

$$\langle \mathbf{u}_p \rangle = \frac{1}{t_f - t_0} \int_{t_0}^{t_f} \left(\frac{1}{N_p} \sum_{i=1}^{N_p} \mathbf{u}_p^{(i)}(t) \right) dt, \quad (2.15)$$

where the stationary period is bounded by t_0 and t_f .

Fluctuations about particle-phase quantities are denoted with two primes, e.g.,

$\mathbf{u}_p'' = \mathbf{u}_p - \langle \mathbf{u}_p \rangle_p$, with $\langle \mathbf{u}_p'' \rangle_p = 0$. Fluctuations from fluid-phase quantities are denoted with three primes, e.g., $\mathbf{u}_f''' = \mathbf{u}_f - \langle \mathbf{u}_f \rangle_f$.

Using this definition, Reynolds stress tensors arise, one in each of the particle and fluid phases, $\langle \mathbf{u}_p'' \mathbf{u}_p'' \rangle_p$ and $\langle \mathbf{u}_f''' \mathbf{u}_f''' \rangle_f$, respectively. These tensors yield the turbulent kinetic energy in the particle and fluid phases. The PA particle-phase and fluid-phase kinetic energies are then defined as,

$$k_p = \frac{1}{2} \langle \mathbf{u}_p'' \cdot \mathbf{u}_p'' \rangle_p \quad (2.16)$$

$$k_f = \frac{1}{2} \langle \mathbf{u}_f''' \cdot \mathbf{u}_f''' \rangle_f. \quad (2.17)$$

In addition to the phase-wise Reynolds stresses, it is also important to note that the Reynolds average of the inner product of the particle velocity fluctuations gives way to the total energy fluctuations in the particle-phase, or the total granular energy, κ_p , given by

$$\kappa_p = \frac{1}{2} \langle \mathbf{u}_p' \cdot \mathbf{u}_p' \rangle. \quad (2.18)$$

Here, angled brackets denote a Reynolds decomposition according to

$\mathbf{u}_p = \langle \mathbf{u}_p \rangle + \mathbf{u}'_p$, with a single prime denoting a fluctuation from the Reynolds-Averaged quantity.

When comparing the particle turbulent kinetic energy, k_p , and the total granular energy, κ_p , it is observed that there is an additional term that represents the uncorrelated, random component of the total particle energy that exists at the particle scale. This is the information that is lost when filtering Lagrangian particle data to the Eulerian mesh to evaluate k_p and is termed ‘granular temperature’, Θ . This yields an expression for the total granular energy,

$$\kappa_p = k_p + \frac{3}{2} \langle \Theta \rangle_p, \quad (2.19)$$

which is equal to the sum of the correlated and uncorrelated contributions, k_p and $3\langle \Theta \rangle_p/2$.

It is notable that in the case of the particle-phase averages, Lagrangian particle quantities, such as $\mathbf{u}_p$, must be evaluated on the Eulerian mesh. This is done by tri-linear interpolation and the application of a Laplacian filter kernel, as defined in Section 2.0.1.3. The projection and filtering of a Lagrangian quantity to the Eulerian grid is denoted as $\tilde{\cdot}$. Thus, the fluctuations about the particle-phase average in an Eulerian sense are defined as,

$$\tilde{\mathbf{u}}''_p = \tilde{\mathbf{u}}_p - \langle \tilde{\mathbf{u}}_p \rangle_p. \quad (2.20)$$

The PA filtered particle-phase and fluid-phase kinetic energy are then defined as

$$k_p = \frac{1}{2} \langle \tilde{\mathbf{u}}_p'' \cdot \tilde{\mathbf{u}}_p'' \rangle_p \quad (2.21)$$

$$k_f = \frac{1}{2} \langle \tilde{\mathbf{u}}_f''' \cdot \tilde{\mathbf{u}}_f''' \rangle_f. \quad (2.22)$$

For fully developed gravity-driven flow, fluid-phase variables are statistically stationary. The fluid-phase continuity equation implies α_f is constant. Further, the fluid-phase momentum equation reduces to $\langle u_f \rangle_f = 0$. Taking the phase average of Eq. (2.6) projected onto the Eulerian mesh yields the particle-fluid-phase momentum equation. The x direction component of this expression, the only non-zero component, is given as

$$\frac{\partial \langle u_p \rangle_p}{\partial t} = \frac{1}{\tau_p^*} (\langle u_f \rangle_p - \langle u_p \rangle_p) + \frac{1}{\rho_p} \left(\left\langle \frac{\partial \tau_{f,xi}}{\partial x_i} \right\rangle_p - \left\langle \frac{\partial p_f}{\partial x} \right\rangle_p \right) + g. \quad (2.23)$$

Here, the transport of the fluid-phase particle velocity results in a balance between the forces exchanged by the fluid (i.e., drag model and resolved surface stresses) and gravity. Prior work [73, 80] has shown that the fluid stress and fluid pressure gradient terms are small enough in gas-solid flows to be reasonably neglected. This implies that at steady state, $\langle u_p \rangle_p \approx \langle u_f \rangle_p + \tau_p^* g$. Here, $\langle u_f \rangle_p$ is often thought of as the fluid velocity *seen by the particles*. Nonlinearities associated with the drag in $\tau_p^* = \langle \tau_p \rangle / \langle F_d \rangle_p$, where $\langle F_d \rangle_p(\langle \alpha_f \rangle, \langle Re_p \rangle)$ is the nonlinear drag correction used as an argument to Eq. (2.8), are

incorporated. These quantities will be leveraged in the following discussions and are utilized to propose models that capture polydisperse effects for both clustering and settling behavior.

2.0.1.5 MODELING ASSUMPTIONS The objective of this work is to isolate the particle-scale and mesoscale mechanisms governing particle settling, clustering, and CIT within PDCs. Resolving these processes throughout an entire PDC is computationally expensive because of the large range of spatial and temporal scales involved. Instead, this work considers a small, statistically representative volume of a PDC, allowing the underlying particle-fluid interactions to be resolved while maintaining computational feasibility.

To make this problem computationally feasible while retaining the dominant physical mechanisms governing settling and clustering, several simplifying assumptions are introduced. The flow is assumed to be isothermal, with constant fluid density and viscosity, allowing the effects of thermal gradients and compressibility to be neglected so that the analysis focuses solely on particle-fluid dynamics. Atmospheric effects, including wind, humidity, and large-scale entrainment, are also neglected because the objective is to investigate local settling behavior rather than the transport and dispersion of an entire PDC. Particles are modeled as rigid spheres with a uniform material density, and only a limited range of particle diameters and volume fractions is considered. These assumptions reduce the complexity associated with irregular particle shapes and variable material

properties while still capturing the dominant mechanisms governing particle settling, clustering, and interphase momentum exchange. Finally, the computational domain represents a small, statistically representative element of a PDC and is simulated over time rather than over the full runout distance. Large-scale phenomena such as topographic interactions, flow front dynamics, and depositional evolution are not resolved, allowing computational resources to be concentrated on the particle-scale and mesoscale processes that are the primary focus of this work.

2.1 COMPUTATIONAL IMPLEMENTATION

All simulations presented in this dissertation were performed using the high-performance computing (HPC) cluster, Matilda, located at Oakland University. The NGA solver was compiled and executed in parallel using the Message Passing Interface (MPI), allowing the computational domain to be decomposed among multiple processors. Particle information was communicated between neighboring processors through ghost cells, enabling efficient parallel execution while maintaining consistency between the Eulerian fluid solver and the Lagrangian particle solver. This parallel implementation significantly reduced the computational cost associated with large particle-laden simulations and allowed substantially larger domains to be simulated than would be practical on a single processor.

The computational cost of each simulation depends primarily on the number of Eulerian grid cells, the number of Lagrangian particles, and the total physical simulation time. Increasing the number of particles not only increases the cost of integrating the

particle equations of motion but also increases the cost associated with collision detection, particle-fluid interpolation, filtering, and interprocessor communication. Likewise, increasing the grid resolution results in a larger system of fluid equations that must be solved at each timestep. Consequently, the simulations presented throughout this dissertation required substantial computational resources and parallel execution to achieve statistically converged solutions.

Simulation output was written periodically throughout each run for subsequent analysis. All post-processing was performed in MATLAB using custom analysis routines developed for this work. These routines were used to compute particle settling statistics, particle clustering metrics, granular temperature, Reynolds stresses, filtered quantities, probability density functions, and other ensemble-averaged statistics discussed in the following chapters.

Each simulation utilized 12 computational nodes, with 40 CPU cores per node, for a total of 480 CPU cores. Individual simulations required approximately four weeks of wall-clock time to complete. This computational cost was incurred for every simulation configuration investigated throughout this work.

CHAPTER 3

SETTLING AND CLUSTERING BEHAVIOR OF PYROCLASTIC DENSITY CURRENTS

3.1 INTRODUCTION

In this chapter, high-fidelity E-L simulations were conducted to investigate particle clustering and settling behavior in polydisperse particle-laden flows. The resulting analyses were used to develop new *a priori* predictors and closure relationships for unresolved multiphase processes. The following sections describe the simulation methodology, including the quantities of interest, followed by an analysis of the steady-state clustering and settling behavior of two polydisperse (i.e., Dist. A and B) and two monodisperse (i.e., Dist. A_0 and B_0) particle distributions, each considered at two particle volume fractions (i.e., $\langle \alpha_p \rangle = 0.01$ and $\langle \alpha_p \rangle = 0.10$).

3.2 METHODOLOGY

3.2.1 SYSTEM DESCRIPTION

The material properties and particle size distributions considered in this study were selected to be representative of the intermediate region of a PDC. The particle density was held constant across all configurations and is consistent with values reported in the literature [12, 100]. Two lognormal particle size distributions, based on the field measurements of Lube et al. [102], were considered, corresponding to $(\phi, \phi_{\text{sorting}}) = (0, 1)$ and $(1.5, 1)$ (see Appendix A for definitions of ϕ and ϕ_{sorting}). These distributions are

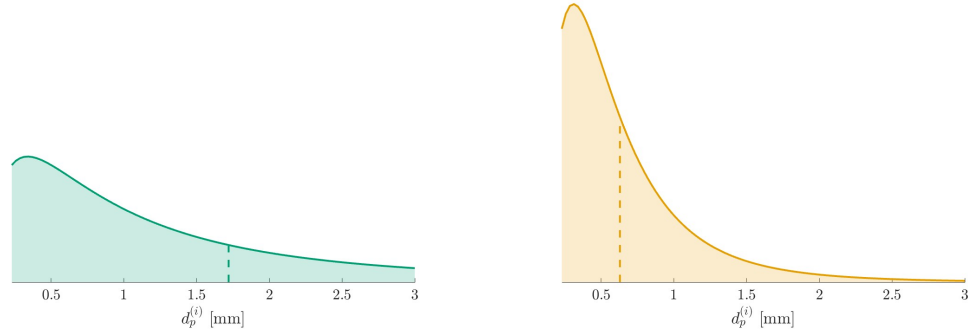
denoted as Dist. A and Dist. B throughout this dissertation. To investigate the influence of particle loading, each distribution was simulated at two global particle-phase volume fractions representative of the intermediate region of a PDC, $\langle \alpha_p \rangle = 0.01$ and 0.10 [6, 11–13, 100, 193]. Here, α_p is defined as the ratio of the volume occupied by particles to the total domain volume, and angled brackets denote a volume-averaged quantity.

It is important to note that the particle diameters for each configuration are selected from the described distribution between the values of $d_{\min}$ and $d_{\max}$. Therefore, the resulting mean and standard deviation deviate from the theoretical mean and standard deviation for a lognormal distribution described by the given μ and σ , since the theoretical mean and standard deviation use infinite support.

Considering two particle distributions and two volume fractions yields four configurations of polydisperse particle assemblies. For each of these, comparisons are drawn with a monodisperse analog, denoted as A_0 and B_0 , where the diameter of the particles in each of these is equivalent to the D_{10} mean diameter of distributions A and B , respectively (for more information on statistical mean diameters, refer to Appendix B).

For gravity-driven gas-solid flows, several relevant non-dimensional quantities emerge. These include the particle Reynolds number, Re_p (*a priori*), defined as $\mathcal{V}_0 d_p / \nu_f$, where $\mathcal{V}_0$ is the Stokes settling velocity for a given particle diameter, defined as $\mathcal{V}_0 = \tau_p g$. The value of Re_p that is reported in Table 3.1 corresponds to that of the $D_{10} = \langle d_p \rangle$ mean particle diameter and is denoted as $\text{Re}_{p,10}$. Likewise, all other quantities that include the subscript ‘10’ imply that the arithmetic mean, $d_{p,10}$, is used for the particle diameter. A list

Table 3.1: Summary of simulation parameters under consideration. The PDFs shown above the table represent the distribution from which particles were sampled and are specified according to lognormal parameters μ and σ . The dashed vertical lines represent the diameter for the corresponding monodisperse simulations.



Distribution A

Distribution B

Polydisperse particle-phase properties					
			Distribution <i>A</i>	Distribution <i>B</i>	
lognormal parameters	μ		0.00	-0.69	
	σ		1.04	0.69	
skewness	$\text{skew}(d_p)$		0.8	1.8	
kurtosis	$\text{kurt}(d_p)$		2.8	7.1	
cut off diameters	$d_{\min}$	[mm]	0.23	0.23	
	$d_{\max}$	[mm]	3.00	3.00	
arithmetic mean diameter	$d_{p,10} = \langle d_p \rangle$	[mm]	1.11	0.69	
standard deviation	$\sqrt{\langle d_p^2 \rangle}$	[mm]	0.70	0.43	
particle relaxation time	$\tau_{p,10}$	[s]	9.47	3.61	
Stokes settling velocity	$\mathcal{V}_{0,10}$	[m/s]	-0.15	-0.06	
Particle Reynolds number	$\text{Re}_{p,10}$		4.83	1.14	
Froude Number	Fr_{10}		1.3×10^3	3.0×10^2	
volume fraction	$\langle \alpha_p \rangle$		(0.01, 0.1)	(0.01, 0.1)	
Number of particles	N_p		(19 627, 198 369)	(75 695, 747 431)	
Monodisperse particle-phase properties					
			Distribution <i>A</i> ₀	Distribution <i>B</i> ₀	
particle diameter	d_p	[mm]	1.72	0.64	
particle relaxation time	τ_p	[s]	22.74	3.12	
Stokes settling velocity	$\mathcal{V}_0$	[m/s]	-0.38	-0.05	
Particle Reynolds number	Re_p		18.00	0.91	
Froude Number	Fr		4.9×10^3	2.5×10^2	
volume fraction	$\langle \alpha_p \rangle$		(0.01, 0.1)	(0.01, 0.1)	
Number of particles	N_p		(12 790, 127 898)	(251 876, 2 518 757)	
Distribution independent properties					
fluid density	ρ_f	[kg/m ³]	0.5		
fluid dynamic viscosity	μ_f	[kg/(m s)]	1.85×10^{-5}		
particle density	ρ_p	[kg/m ³]	2500		
gravity	$\mathbf{g}$	[m/s ²]	(-0.016, 0, 0)		
<i>a priori</i> mass loading	φ_0		(50.27, 552.7)		
Domain size	$L_x \times L_y \times L_z$	[mm]	(603.7 × 75.10 × 75.10)		

of these non-dimensional numbers and other important simulation parameters are summarized in Table 3.1.

A domain size of $2.90\mathcal{L} \times 0.36\mathcal{L} \times 0.36\mathcal{L}$ was adopted to balance computational cost with statistical accuracy. The domain is sufficiently large to contain the particle population necessary to produce representative settling and clustering statistics while remaining computationally feasible. To preserve these nondimensional domain dimensions, the gravitational acceleration was adjusted such that the resulting characteristic cluster length matched the physical size of the computational domain. The grid resolution was subsequently selected to adequately resolve the particle clustering statistics while maintaining consistency with the validated monodisperse simulations [73].

3.3 RESULTS

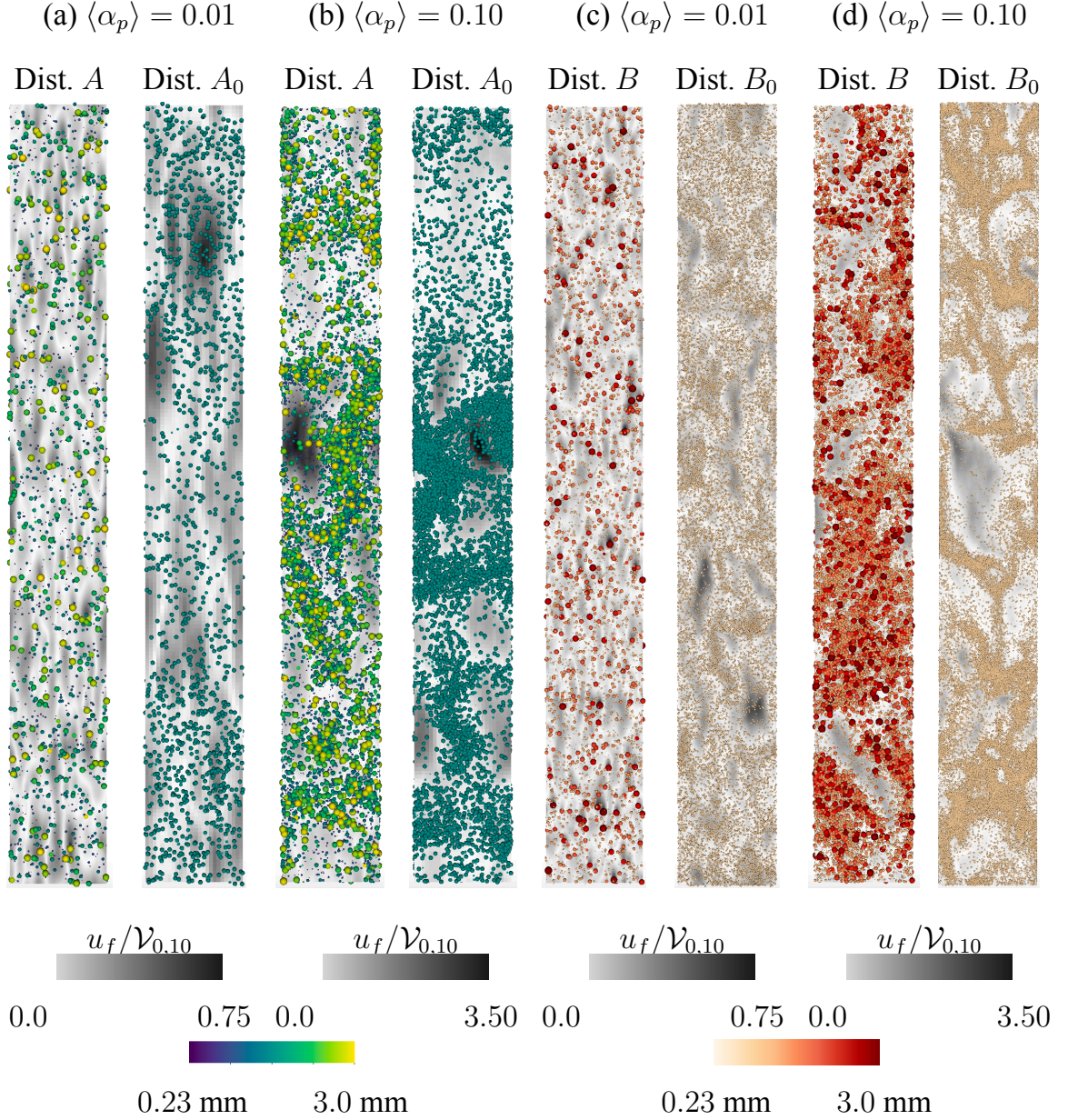


Figure 3.1: Representative snapshots obtained during the statistically stationary period for each configuration. Each image shows an $x-y$ plane at $z = 0$. The fluid-phase velocity, shown in grayscale, is normalized by the polydisperse Stokes settling velocity, $\mathcal{V}_{0,10}$. Particles are colored according to diameter, ranging from blue to yellow for Dist. A and from pink to red for Dist. B.

3.3.1 AN ANALYSIS OF CLUSTERING BEHAVIOR

Before discussing the effects of polydispersity on particle clustering and its influence on settling behavior, the impact of polydispersity on particle packing is first examined.

Representative steady-state slices for each configuration, illustrating both clustering and settling behavior, are shown in Figure 3.1.

3.3.1.1 MAXIMUM RANDOM CLOSE PACKED VOLUME FRACTION It has been previously established that the random close-packed (RCP) volume fraction of monodisperse spheres is $\alpha_{\text{rcp}} = 0.64$ [194–197]. This value represents the maximum achievable volume fraction for a randomly packed arrangement of spheres. While close packing efficiencies for polydispersed assemblies of spheres are less established in comparison, several theoretical and computational studies have quantified the RCP efficiency for lognormal distributions of spheres [194–197]. Farr [194] proposed an algorithm that maps 3D configurations of spheres onto a 1D system of rods. This method has shown success in accurately and efficiently estimating the RCP efficiency of lognormally distributed spheres. This approach, known as the rod packing (RP) algorithm [194], was subsequently validated [195] and yielded a closed-form expression (Eq. (3.2)). It was observed that the RCP efficiency depended only on a measure of the distribution's width, denoted $\tilde{\sigma}$ [195]. This parameter is computed using the ratio of the

volume moment diameter to the surface moment diameter as

$$\tilde{\sigma} = \sqrt{\ln \left(\frac{d_{4,3}}{d_{3,2}} \right)}. \quad (3.1)$$

An alternative way to characterize the particle size distribution is through the diameter $d_{4,3}$, which emphasizes the particle sizes that contribute most to the total particle volume and is therefore more sensitive to large particles. In contrast, the diameter $d_{3,2}$, defined as the diameter of a monodisperse assembly of N_p particles with the same volume-to-surface-area ratio as the polydisperse assembly, places more weight on small particles and is thus more sensitive to the fine particles.

Due to this, larger values of $\tilde{\sigma}$ are indicative of distributions containing a greater number of very small particles. The model relating α_{rcp} to $\tilde{\sigma}$ based on results of the RP algorithm [195] is given as

$$\alpha_{\text{rcp}}(\tilde{\sigma}) = 1 - 0.57e^{-\tilde{\sigma}} + 0.2135e^{\frac{-0.57\tilde{\sigma}}{0.2135}} + 0.0019(\cos(2\pi(1 - e^{-0.75\tilde{\sigma}^{0.7} - 0.025\tilde{\sigma}^4})) - 1). \quad (3.2)$$

The RCP efficiency based on $\tilde{\sigma}$ for each of the lognormal distributions under study is summarized in Table 3.2.

While both volume fractions, each for Distributions *A* and *B*, were sampled from the same lognormal distribution, the number of discrete particles in the systems differed (fewer for $\langle \alpha_p \rangle = 0.01$ compared with $\langle \alpha_p \rangle = 0.10$). As expected, there are minimal

Table 3.2: Summary of the arithmetic mean, surface area, volume, Sauter and volume moment mean diameters, distribution width, $\tilde{\sigma}$, and maximum random close packing efficiency resulting from Eq. (3.2) for the particles studied in each configuration.

		Distribution A		Distribution B	
		<i>volume fraction, $\langle\alpha_p\rangle$</i>			
		<i>0.01</i>	<i>0.10</i>	<i>0.01</i>	<i>0.10</i>
$d_{1,0}$	[mm]	1.11	1.11	0.68	0.68
$d_{2,0}$	[mm]	1.31	1.31	0.81	0.81
$d_{3,0}$	[mm]	1.49	1.48	0.95	0.95
$d_{3,2}$	[mm]	1.91	1.91	1.30	1.31
$d_{4,3}$	[mm]	2.16	2.15	1.65	1.65
$\tilde{\sigma}$	[–]	0.3483	0.3499	0.4824	0.4810
α_{rcp}	[–]	0.6793	0.6796	0.7038	0.7036

differences in the statistical descriptions between the two volume fractions because the lognormal distribution for particle size is the same for each distribution at the dilute and dense volume fractions.

As one might anticipate, the lognormally distributed particles exhibit a higher maximum RCP volume fraction, as small particles in the distribution occupy voids that would otherwise remain in a monodisperse packing arrangement of particles with a diameter equal to the mean particle diameter. Visualizations for the RCP efficiencies for Distributions A , B , A_0 and B_0 are shown, along with their associated α_{rcp} in Figure 3.2. As expected, the RCP efficiency of Dist. B at dilute volume fraction, $\alpha_{\text{rcp}}^B = 0.7038$, provides the largest RCP and is used as the normalization factor for volume fraction when computing quantities of interest in this study.

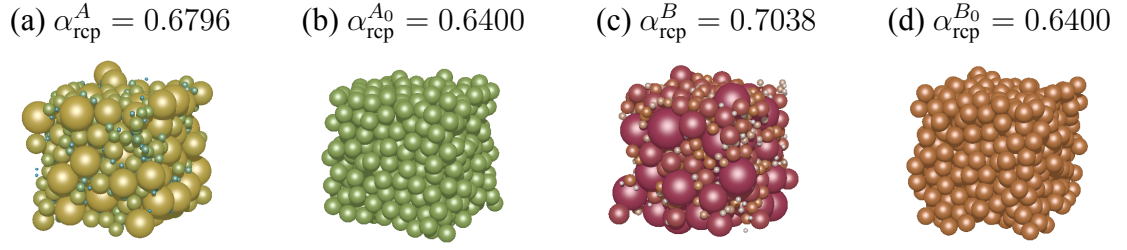


Figure 3.2: Random close-packed configurations for the configurations under study. Here α_{rcp} denotes the RCP volume fraction from the RP algorithm. Visualizations generated by the Kansal Torquato Stillinger (KTS) algorithm [197] and RP software [195].

Values reported in Table 3.2 are the random close-packing efficiency limits for the *entire* collection of particles. As the flow reaches a statistically stationary state and particles become increasingly correlated, clusters spontaneously form. Notably, particles within clusters do not necessarily mirror the overall particle distribution. If larger particles are more likely to be found in clusters than smaller particles, then the close-packing efficiency of the subset of particles involved in a cluster will differ from what would be expected for an assembly representative of the full domain.

The packing efficiency of particles influences their behavior within a fluid flow. The occurrence of larger clusters is enhanced when particles are efficiently packed or closely arranged. That said, the reported results depend on the number of particles in the distribution. Distribution *A* has significantly fewer particles than Distribution *B*. The likelihood of particles making contact with one another, therefore, decreases.

3.3.1.2 STATISTICALLY STATIONARY ANALYSIS ON CLUSTERING The deviation of the volume fraction in a random distribution of particles is often used to characterize the mean degree of clustering, with the parameter $\mathcal{D}$ introduced by Eaton and Fessler [198].

$$\mathcal{D} = \frac{\left(\sqrt{\langle \alpha_p'^2 \rangle} - \sqrt{\langle \alpha_p'^2 \rangle}_0 \right)}{\langle \alpha_p \rangle} \approx \frac{\sqrt{\langle \alpha_p'^2 \rangle}}{\langle \alpha_p \rangle}, \quad (3.3)$$

Where $\langle \alpha_p'^2 \rangle$ is the variance of the particle volume fraction of the fully developed configuration and $\langle \alpha_p'^2 \rangle_0$ is the variance of an uncorrelated assembly of particles, assumed here to be null. As a collection of particles becomes increasingly correlated and heterogeneity in the flow develops, this quantity similarly increases. This parameter $\mathcal{D}$ is computed for each case considered in this study and is summarized in Table 3.3.

Although mean-variance in volume fraction has been used and validated for monodisperse particle assemblies, it is agnostic to particle-size distribution. The third and fourth moment means of the filtered particle-phase volume fraction are also relevant for characterizing the extent of clustering. These quantities are tabulated in Table 3.3 for each of the configurations and are defined as

$$\text{skew}(\alpha_p) = \frac{\sum_{i=1}^{N_{\text{cells}}} \left(\alpha_p^{(i)} - \langle \alpha_p \rangle \right)^3}{(N_{\text{cells}} - 1) (\text{var}(\alpha_p))^{3/2}} \quad (3.4)$$

$$\text{kurt}(\alpha_p) = \frac{\sum_{i=1}^{N_{\text{cells}}} \left(\alpha_p^{(i)} - \langle \alpha_p \rangle \right)^4}{(N_{\text{cells}} - 1) (\text{var}(\alpha_p))^2}. \quad (3.5)$$

Table 3.3: Summary of surface loading and statistics on volume fraction for all configurations under study.

$\langle \alpha_p \rangle$	Dist.	$\mathcal{S}$	$\mathcal{D}$	$\text{skew}(\alpha_p)$	$\text{kurt}(\alpha_p)$
0.01	A_0	2.07	0.42	0.66	3.37
	A	1.21	0.87	2.81	15.69
	B_0	0.28	0.49	0.82	3.90
	B	0.46	1.34	6.50	80.68
0.10	A_0	2.28	0.68	1.62	5.79
	A	1.32	0.69	1.74	7.62
	B_0	0.31	0.80	1.55	5.95
	B	0.51	0.78	1.50	5.62

Skewness represents the asymmetry of a distribution, with $\text{skew}(\alpha_p) = 0$ denoting a normal distribution. Positive values of skewness imply that the distribution is skewed towards very dense particle distributions. Conversely, a negative skewness indicates a very dilute particle distribution. Kurtosis is a measure of the ‘tailedness’ of the distribution and indicates how the volume fraction is distributed between the mean and tails. Kurtosis helps us understand whether the data has a heavy tail (more extreme outliers) or a light tail, which is seen in a normal distribution. Positive (leptokurtic) and negative (platykurtic) values represent distributions that are more tightly and more loosely spread about the mean, respectively.

The variance in volume fraction is substantially higher in dilute polydisperse configurations relative to their monodisperse counterparts. In particular, the ratios of the standard deviation for Dist. A/A_0 and B/B_0 are 2.07 and 2.73, respectively. This trend is consistent with a larger skewness and kurtosis seen in the polydisperse distributions compared to their monodisperse analogs. The standard deviation in particle volume

fraction is nearly equivalent between the polydisperse configurations and their monodisperse counterparts at high volume fraction. The difference between A and A_0 is 1.40%, and the difference between B and B_0 is 2.50%. A similar trend is observed when considering the skewness and the kurtosis in the particle volume fraction. As expected, the polydisperse configurations have larger skewness than their monodisperse counterparts. In the dilute suspension, the presence of larger particles plays a greater role in reducing drag. When particles are polydisperse, the presence of a larger particle creates a large region of reduced drag, leading to larger regions of clustering (quantified in Section 3.3.2). This is why the difference in deviation in volume fraction is larger for the polydisperse configurations at low volume fraction. At high volume fraction, there are sufficient particles in the domain to consistently perturb the flow, producing regions of reduced drag and resulting in particle clustering. Due to the number of particles present, the presence of a larger particle does not play as significant a role in the degree of clustering. Owing to this, the standard deviation in particle volume fraction is nearly equivalent at high volume fraction.

Mass loading given as $(\varphi = \rho_p \langle \alpha_p \rangle / (\rho_f \langle \alpha_f \rangle))$ can be considered as the ratio of the mass of the particles to the mass of the fluid in a given volume of the flow, and has historically been used as an *a priori* estimate for predicting clustering. Mass loading is, by definition, agnostic to how mass is partitioned throughout a volume and, therefore, is insufficient for predicting the degree of clustering in polydisperse flows. The mass loading of all the configurations A , A_0 , B and B_0 is 50.5 at $\langle \alpha_p \rangle = 0.01$ and 555.5 for all

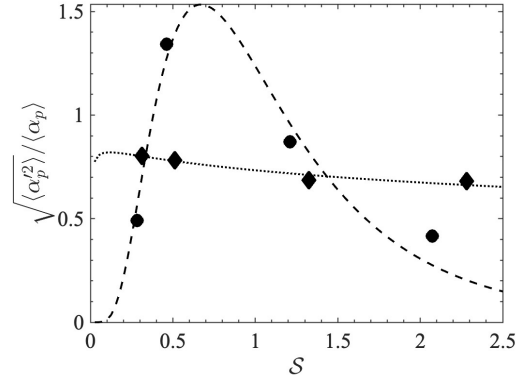


Figure 3.3: Deviation of normalized particle-phase volume fraction as a function of surface loading. Circles represent data for $\langle \alpha_p \rangle = 0.01$ and diamonds represent data for $\langle \alpha_p \rangle = 0.10$. The loosely and densely dashed lines represent the model described in Eq. (3.7) for $\langle \alpha_p \rangle = 0.01$ and 0.10 , respectively.

configurations at $\langle \alpha_p \rangle = 0.10$. This metric is related to $\mathcal{D}$ in the case of monodisperse assemblies of particles (e.g., [73, 80]).

An alternate *a priori* predictor for the degree of clustering expected in polydisperse gas-solid flows is proposed and is referred to as surface loading. This quantity leverages the mean particle surface diameter. For these models, the mean surface diameter was selected because it quantifies which particles most often touch the fluid and which contribute most to surface area.

$$\mathcal{S} = \left(\frac{1}{\langle \alpha_f \rangle A_{\text{cross}}} \right) \left(\frac{\rho_p}{\rho_f} \right) \frac{\pi}{4} \frac{1}{N_p} \underbrace{\sum_{i=1}^{N_p} (d_p^{(i)})^2}_{(D_{30})^3 / D_{32}} \quad (3.6)$$

Where A_{cross} is the area of the cross-stream plane and the term in brackets is the square of the surface mean diameter. The functional form of this equation was selected to be dimensionless and to account for particle separation, whereas mass loading was not.

It can be seen in Figure 3.3 that the dense suspensions' surface loading versus degree of clustering follows a more lognormal curve, whereas the dilute suspensions have similar degrees of clustering. This is a key result as it shows that particle size distribution alone can strongly change clustering behavior. Two systems with the same volume fraction can behave completely differently, and therefore, current models are not accurate.

Owing to this, a model for $\mathcal{D}$ as a function of the surface loading was proposed, shown as dashed lines in Figure 3.3, and defined as

$$\frac{\sqrt{\langle \alpha_p'^2 \rangle}}{\langle \alpha_p \rangle} = \frac{1}{\mathbb{E} \mathcal{S}} \exp \left(\frac{-(\ln(\mathcal{S}) - \mathbb{F})^2}{\mathbb{G}} \right) \quad (3.7)$$

where the coefficients $\mathbb{E}$, $\mathbb{F}$ and $\mathbb{G}$, depend upon the mean volume fraction as,

$$\mathbb{E}(\langle \alpha_p \rangle) = -8.2\langle \alpha_p \rangle + 0.9 \quad (3.8)$$

$$\mathbb{F}(\langle \alpha_p \rangle) = 76.0\langle \alpha_p \rangle - 0.8 \quad (3.9)$$

$$\mathbb{G}(\langle \alpha_p \rangle) = 164.0\langle \alpha_p \rangle - 0.9. \quad (3.10)$$

The coefficients $\mathbb{E}$, $\mathbb{F}$, and $\mathbb{G}$ were determined using ordinary least-squares (OLS) regression based on the simulation data. The functional form of Eq. (3.7) was selected to reproduce the observed non-monotonic dependence of particle clustering on the surface loading parameter, $\mathcal{S}$, while enforcing the expected asymptotic behavior. As $\mathcal{S} \rightarrow 0$ or $\mathcal{S} \rightarrow \infty$, particle clustering diminishes and the normalized particle volume fraction

fluctuations approach zero. Between these limits, clustering reaches a finite maximum at an intermediate value of $\mathcal{S}$, consistent with the simulation results. The resulting relationship is therefore semi-empirical, with the regression determining only the coefficient values while the functional form prescribes the physically motivated trends. Consequently, the model should be applied only within the range of particle volume fractions and surface loadings considered in this study.

Because only two mean particle volume fractions were simulated, the dependence of $\mathbb{E}$, $\mathbb{F}$, and $\mathbb{G}$ on $\langle\alpha_p\rangle$ was assumed to be linear, representing the simplest relationship supported by the available data. Additional simulations spanning a broader range of particle volume fractions are needed to determine whether higher-order dependencies are warranted. Furthermore, previous work by Beetham et al. [80] suggests that particle clustering also depends on the Archimedes (or equivalently Froude) number, a dependence that is not captured by the surface loading parameter, $\mathcal{S}$, alone.

Several other mean quantities are important for describing the bulk behavior of gas-solid flows, including the mean settling velocity, $\langle u_p \rangle$. The normalized mean settling velocity is larger for the polydisperse configurations and is more pronounced when $\langle\alpha_p\rangle = 0.01$. As shown in Figure 3.4 (a), the dilute configurations show a stronger correlation to the degree of clustering, $\mathcal{D}$. Configurations with $\langle\alpha_p\rangle = 0.10$ exhibit a wider range of settling velocities for a narrower range of $\mathcal{D}$.

A mathematical relationship between surface loading and normalized mean settling velocity is shown in Eq. (3.11), where $\mathbb{H} = 0.15$ and $\mathbb{I} = 0.8$. Notably, the

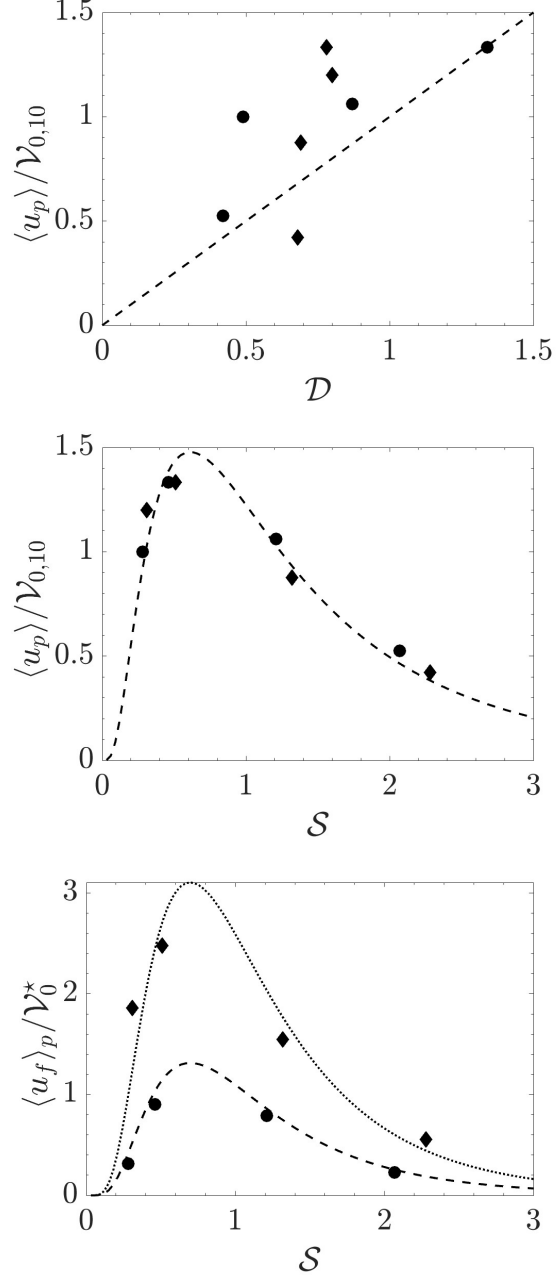


Figure 3.4: Summary of the normalized mean settling velocity with respect to (a) degree of clustering, $\mathcal{D}$, and (b) surface loading $\mathcal{S}$. The normalized contribution of $\langle u_f \rangle_p$ relative to $\mathcal{S}$ is shown in (c). Configurations with $\langle \alpha_p \rangle = 0.01$ are denoted with solid circles, and configurations with $\langle \alpha_p \rangle = 0.10$ are denoted with solid diamonds. The dashed lines represents a one-to-one correlation in (a) and the model prescribed by Eq. (3.11) in (b) and Eq. (3.13) in (c).

simulation data collapse onto a single curve for both particle volume fractions considered in this work, resulting in constant values for the coefficients $\mathbb{H}$ and $\mathbb{I}$.

$$\frac{\langle u_p \rangle}{\mathcal{V}_{0,10}} = \frac{2.5}{(\mathbb{I}\mathcal{S}\sqrt{2\pi})} \exp\left(-\frac{(\ln(\mathcal{S}) - \mathbb{H})^2}{2\mathbb{I}^2}\right) \quad (3.11)$$

The functional form of Eq. (3.11) was selected to reproduce the observed non-monotonic dependence of the normalized mean settling velocity on the surface loading parameter, $\mathcal{S}$, while enforcing the expected asymptotic behavior. As $\mathcal{S} \rightarrow 0$, weak particle-fluid interactions cause the normalized settling velocity to approach zero, whereas as $\mathcal{S} \rightarrow \infty$, particle-particle interactions suppress settling enhancement, again causing the normalized settling velocity to approach zero. Consequently, the model predicts a finite maximum at an intermediate value of $\mathcal{S}$, consistent with the simulation results. The resulting model data can be seen in Figure 3.4 (b).

As was previously discussed in Section 2.0.1.4, the mean settling velocity can also be expressed as

$$\langle u_p \rangle = \langle u_f \rangle_p + \mathcal{V}_0^*, \quad (3.12)$$

where $\mathcal{V}_0^*$ is defined as $\tau_p^* g$ with $\tau_p^* = \tau_p / F_d$, and mean flow quantities, $\langle d_p \rangle$ and $\langle \alpha_p \rangle$, are used as arguments to the previously defined expressions for the settling time and drag correction factor.

In this expression, $\mathcal{V}_0^*$ is known, while a model is required for $\langle u_f \rangle_p$. The relative contribution of the fluid-phase velocity to the mean settling velocity is approximately 2.4

times larger for the higher particle volume fraction configurations. A semi-empirical model, motivated by the observed dependence on surface loading, is proposed,

$$\frac{\langle u_f \rangle_p}{\mathcal{V}_0^*} = \frac{\mathbb{J}}{0.6\mathcal{S}\sqrt{2\pi}} \exp\left(-\frac{(\ln(\mathcal{S}))^2}{2\mathbb{I}^2}\right) + 1, \quad (3.13)$$

where the coefficient $\mathbb{J}$ is 1.65 and 3.9 for $\langle \alpha_p \rangle = 0.01$ and 0.10, respectively.

The functional form of Eq. (3.13) was selected to reproduce the observed dependence of the fluid-phase velocity sampled by the particles on the surface loading parameter, $\mathcal{S}$, while enforcing the expected asymptotic behavior. As $\mathcal{S} \rightarrow 0$ and $\mathcal{S} \rightarrow \infty$, the normalized sampled fluid velocity approaches its baseline value, indicating that particle-fluid interactions provide no additional enhancement. Between these limits, the model predicts a finite maximum at an intermediate value of $\mathcal{S}$, consistent with the simulation results.

The coefficient $\mathbb{J}$ was determined using ordinary least-squares (OLS) regression, while the functional form prescribes the observed trends and physically expected limiting behavior. Consequently, the proposed relationship is semi-empirical and is valid over the range of particle volume fractions and surface loadings considered in this study.

Additional simulations spanning a broader range of particle volume fractions are required to determine whether this dependence is linear or nonlinear. The resulting model data can be seen in Figure 3.4 (c).

Table 3.4: Summary of the domain mean settling velocities and contributions from $\langle u_f \rangle_p$ and $\mathcal{V}_0^*$ along with the relative contributions to total granular energy from particle-phase TKE and granular temperature as well as the relative magnitude of fluid-phase TKE relative to granular energy.

$\langle \alpha_p \rangle$	Dist.	$\langle u_p \rangle$ [m/s]	$\mathcal{V}_0^*$ [m/s]	$\langle u_f \rangle_p$ [m/s]	$\frac{\langle u_f'^2 \rangle}{k_f}$	$\frac{\langle v_f'^2 \rangle}{k_f}$	$\frac{\langle u_p'^2 \rangle}{k_p}$	$\frac{\langle v_p'^2 \rangle}{k_p}$	$\frac{k_f}{\kappa_p}$	$\frac{k_p}{\kappa_p}$	$\frac{3\langle \Theta \rangle_p}{(2\kappa_p)}$	St_η	Re_γ
0.01	A_0	-0.20	-0.16	-0.04	1.89	0.05	1.76	0.06	4.29	0.34	0.66	0.28	4.09×10^3
	A	-0.17	-0.10	-0.07	1.88	0.06	1.54	0.35	1.04	0.20	0.79	0.03	2.44×10^4
	B_0	-0.05	-0.04	-0.01	1.66	0.17	1.71	0.22	3.89	0.48	0.52	0.01	2.00×10^3
	B	-0.08	-0.04	-0.04	1.77	0.13	1.47	0.11	0.81	0.29	0.71	0.02	7.74×10^3
0.10	A_0	-0.16	-0.10	-0.06	1.64	0.21	1.60	0.17	12.40	0.67	0.33	0.81	1.20×10^4
	A	-0.14	-0.05	-0.09	1.68	0.17	11.84	0.17	13.18	0.67	0.33	0.06	1.10×10^5
	B_0	-0.06	-0.02	-0.04	1.53	0.20	2.01	0.23	5.57	0.81	0.19	0.06	1.31×10^5
	B	-0.08	-0.02	-0.06	1.54	0.18	1.82	0.20	8.18	0.71	0.29	0.03	5.48×10^4

The partitioning of fluctuating energy between the particle and fluid phases depends strongly on both particle size distribution and mean particle volume fraction, as shown in Table 3.4. For the dilute cases, the polydisperse configurations exhibit a larger fraction of their total granular energy in the form of granular temperature than their corresponding monodisperse configurations. This increase is most pronounced for distributions B and B_0 , indicating that broader particle size distributions containing a larger proportion of small particles promote greater random particle motion. Physically, smaller particles are more readily accelerated by the surrounding fluid, leading to increased particle agitation and a larger granular temperature.

As the mean particle volume fraction increases, the contribution of granular temperature to the total granular energy decreases for all particle distributions, while both the fluid-phase and particle-phase turbulent kinetic energies increase. This suggests that increasing particle loading redistributes the fluctuating energy away from random particle motion and toward coherent fluid-particle interactions. The increased frequency of particle interactions at higher volume fractions suppresses random particle fluctuations while simultaneously enhancing momentum exchange with the carrier phase.

Across all configurations, the fluid-phase turbulent kinetic energy exceeds the particle-phase turbulent kinetic energy, indicating that a larger fraction of the fluctuating kinetic energy generated by particle settling resides in the carrier fluid. This observation supports that in CIT, particle clusters transfer momentum to the surrounding fluid through

interphase coupling, generating turbulence that contains more energy than the particle-phase velocity fluctuations themselves.

The decomposition of the mean settling velocity further highlights the importance of particle-fluid interactions. For the dilute configurations, the isolated-particle settling contribution, $\mathcal{V}_0^*$, dominates the mean settling velocity, while the fluid-phase contribution, $\langle u_f \rangle_p$, provides a relatively small correction. As the particle volume fraction increases, however, the fluid-phase contribution becomes comparable to, and in some cases exceeds, the isolated-particle settling velocity. This demonstrates that collective particle-fluid interactions become increasingly important at higher particle concentrations and that the induced fluid motion generated by clustering plays a significant role in determining the overall settling behavior. Consequently, models based solely on isolated-particle settling cannot adequately predict the settling velocity in dense, polydisperse suspensions.

Finally, the Stokes number, St_η , and Taylor Reynolds number, Re_λ , are reported to characterize the particle and fluid dynamics. The Taylor Reynolds number, $Re_\lambda = \frac{u_{rms}\lambda}{\nu_f}$, characterizes the intensity of the fluid turbulence. The values reported in Table 3.4 indicate that all simulations reside within a turbulent regime where inertial effects dominate viscous dissipation, providing conditions favorable for the development of CIT.

3.3.1.3 FINER-GRAINED APPROACH TO CHARACTERIZING CLUSTERING

BEHAVIOR The following section takes a finer-grained approach to characterizing the

clustering behavior of the configurations under study, wherein the flow behavior is examined using a statistical approach as well as proposing improved models.

In this work, ‘clusters’ are identified as regions in the flow corresponding to a particle volume fraction greater than 1.5 times the domain mean, $\langle\alpha_p\rangle$. Additionally, the flow is divided into the following regions:

1. **Region A:** Most dilute regime, $\alpha_p \leq 1.5\langle\alpha_p\rangle$
2. **Region B:** Loosely clustered regime, $1.5\langle\alpha_p\rangle < \alpha_p \leq 2.25\langle\alpha_p\rangle$
3. **Region C:** Moderately clustered regime, $2.25\langle\alpha_p\rangle < \alpha_p \leq 3.0\langle\alpha_p\rangle$
4. **Region D:** Densely clustered regime, $\alpha_p > 3.0\langle\alpha_p\rangle$

These regions will be referred to throughout the dissertation and are shown in designated colors that increase from white (most dilute) to dark gray (most dense).

Representative slices of the domain at a statistically stationary state of each configuration with respect to local volume fraction and contours are plotted following the four-region convention for identifying areas of increasing particle correlation, and normalizing based on the maximum random close-packing efficiency for Distribution B (see Figures 3.5–3.7), as described in 3.3.1.1.

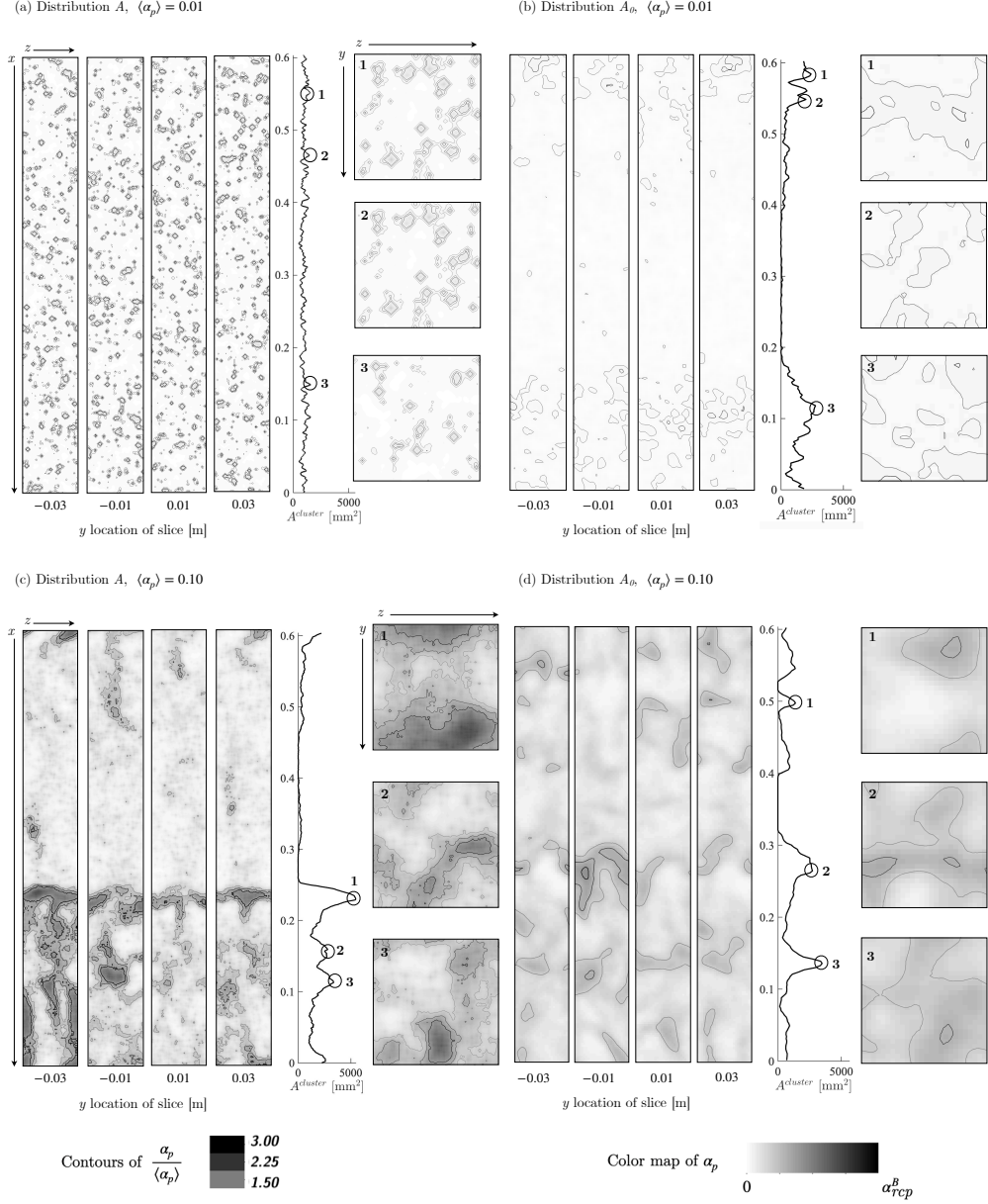


Figure 3.5: Overview of the clustering patterns observed in Distributions A (left figures) and A_0 (right figures) at $\langle \alpha_p \rangle = 0.01$ (top row) and 0.10 (bottom row).

It is shown that, in both volume fraction configurations, the monodisperse cases have smoother contours than their polydisperse analogs and achieve lower packing

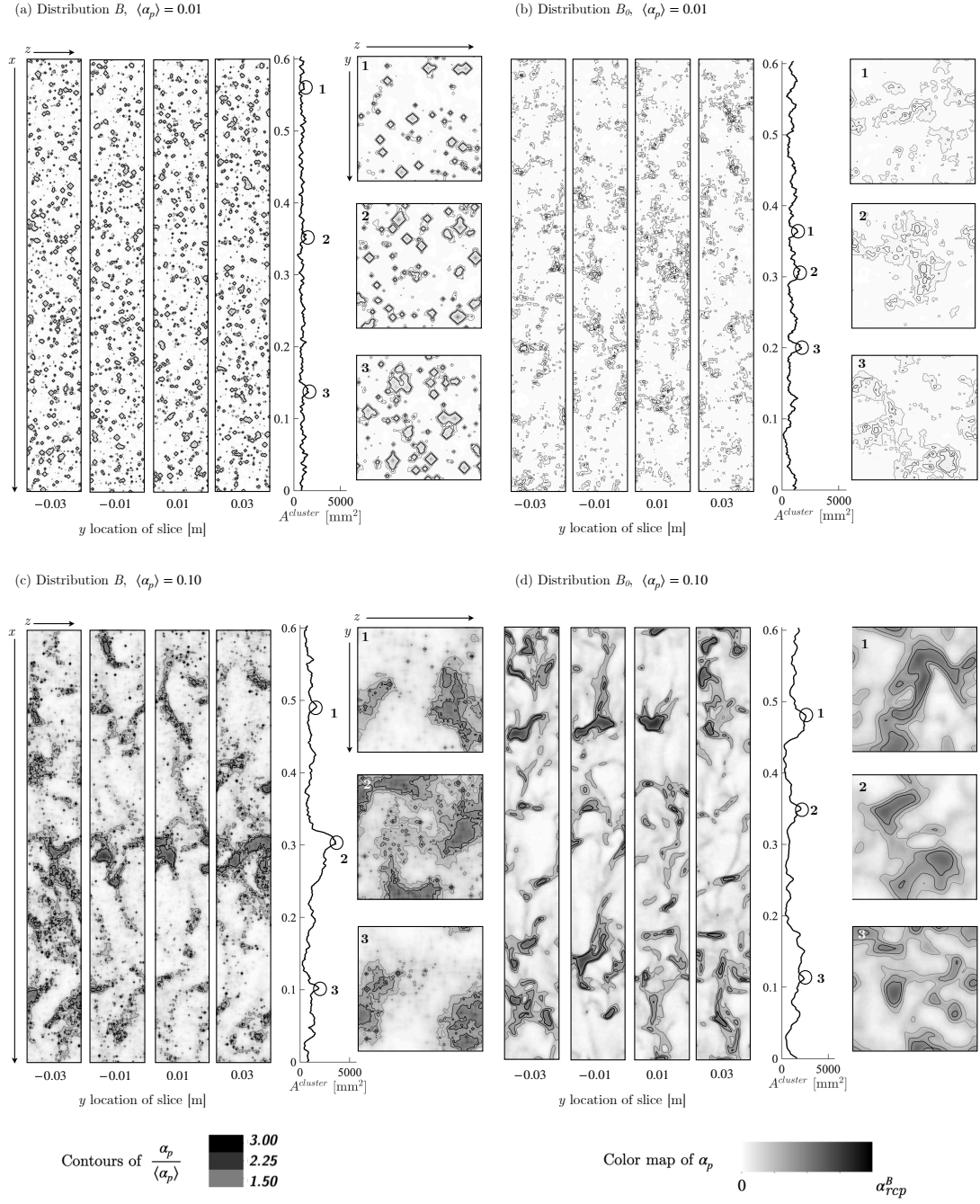


Figure 3.6: Overview of the clustering patterns observed in Distributions B (left figures) and B_0 (right figures) at $\langle \alpha_p \rangle = 0.01$ (top row) and 0.10 (bottom row).

efficiency in their cores. This is due to the increased potential packing efficiency in polydisperse particle assemblies.

Monodisperse configurations with larger mean particle diameters (Distribution A_0) contain larger clusters in comparison to configurations with smaller mean diameters. Distribution B_0 contains a greater number of smaller clusters. The clusters in Dist. B_0 appear to be denser. This is due to differences in the total number of particles in the domain, even though the maximum packing efficiency for a monodisperse assembly of particles is the same.

When comparing each polydisperse configuration with its monodisperse analog, it is observed that the polydisperse configurations contain more small, densely packed clustered regions than their monodisperse counterparts, which exhibit less densely packed clusters more sparsely arranged throughout the domain. At higher volume fraction, cluster shape is similar in the polydisperse and monodisperse configurations. These results are further bolstered by the degree of clustering presented in Table 3.3

The cross-stream composition of clusters is also considered. Shown in Figures 3.5 and 3.6, the total cross-stream clustering area is calculated by summing the number of Eulerian cells containing a local particle volume fraction greater than $1.5\langle\alpha_p\rangle$ and multiplying this value by the $y - z$ area of the cells.

When comparing the cluster cross-sectional area curves for A and A_0 at $\langle\alpha_p\rangle = 0.01$, it is observed that the maximum cluster cross-sectional area is significantly

larger for configuration A_0 . This is supported by the observation that clusters in A_0 are qualitatively larger in size but fewer in number.

Dist. A , clusters are more evenly spread along the streamwise direction than in Dist. A_0 . However, at a higher volume fraction $\langle \alpha_p \rangle = 0.10$, the maximum cluster areas for both Dist. A and A_0 are similar and appear at similar intervals.

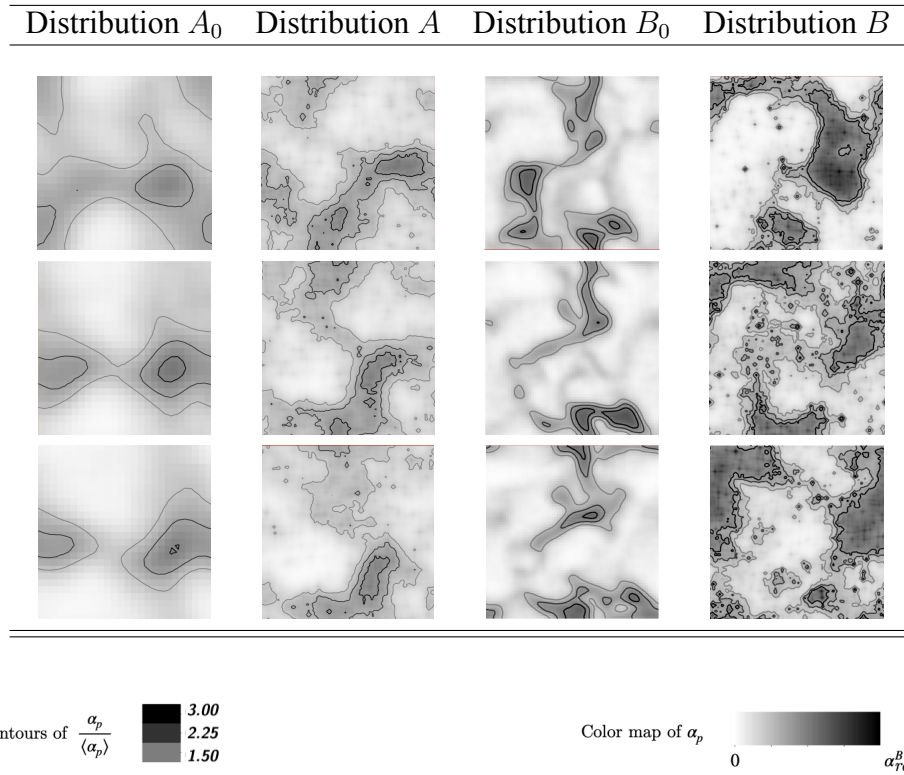


Figure 3.7: Cross sections of particle volume fraction in the $y - z$ plane with contours denoting volume fractions of $(1.5, 2.25, 3.0)\langle \alpha_p \rangle$. The color map represents particle volume fraction and ranges from 0 (white) to α_{rcp} (black). Cross sections are the same as those detailed in Figures 3.5 and 3.6, but are shown together here to aid in comparisons across the configurations studied at $\langle \alpha_p \rangle = 0.10$.

Dist. B and B_0 show similar patterns with a few differences. At a low volume fraction $\langle \alpha_p \rangle = 0.01$, Dist. B_0 has slightly larger peak cluster areas, but these peaks are

spread similarly to those in Dist. *A*. At a higher volume fraction $\langle \alpha_p \rangle = 0.10$, Dist. *B* reaches slightly higher cluster area values than Dist. B_0 , which aligns with the observation that some polydisperse clusters in Dist. *B* are more cross-stream oriented rather than stream-wise.

As detailed in Figure 3.7, the structures of the polydisperse clusters are more fragmented than their monodisperse counterparts. This is partly due to the presence of particles ranging from very small to very large in the domain, but it may also point to the formation of larger clusters when two moderately sized clusters merge. These qualitative observations are consistent with the quantitative results presented in the previous sections, demonstrating that particle size distribution alone dramatically changes clustering structure.

Finally, the distribution of granular temperature is examined. (Figure 3.8 Figure 3.9) within each of the Regions A-D in the flow. The solid lines in Figures 3.8 and 3.9 represent the normalized domain-wide distribution, while the shaded areas indicate the corresponding normalized distributions within each region. All four polydisperse configurations exhibit broadly similar trends. The granular temperature is highest in the most dilute regions of the flow and decreases as the local volume fraction increases. This behavior suggests that particles in dilute zones have greater uncorrelated kinetic energy compared to those embedded within cluster cores and is consistent with the results reported in Table 3.4.

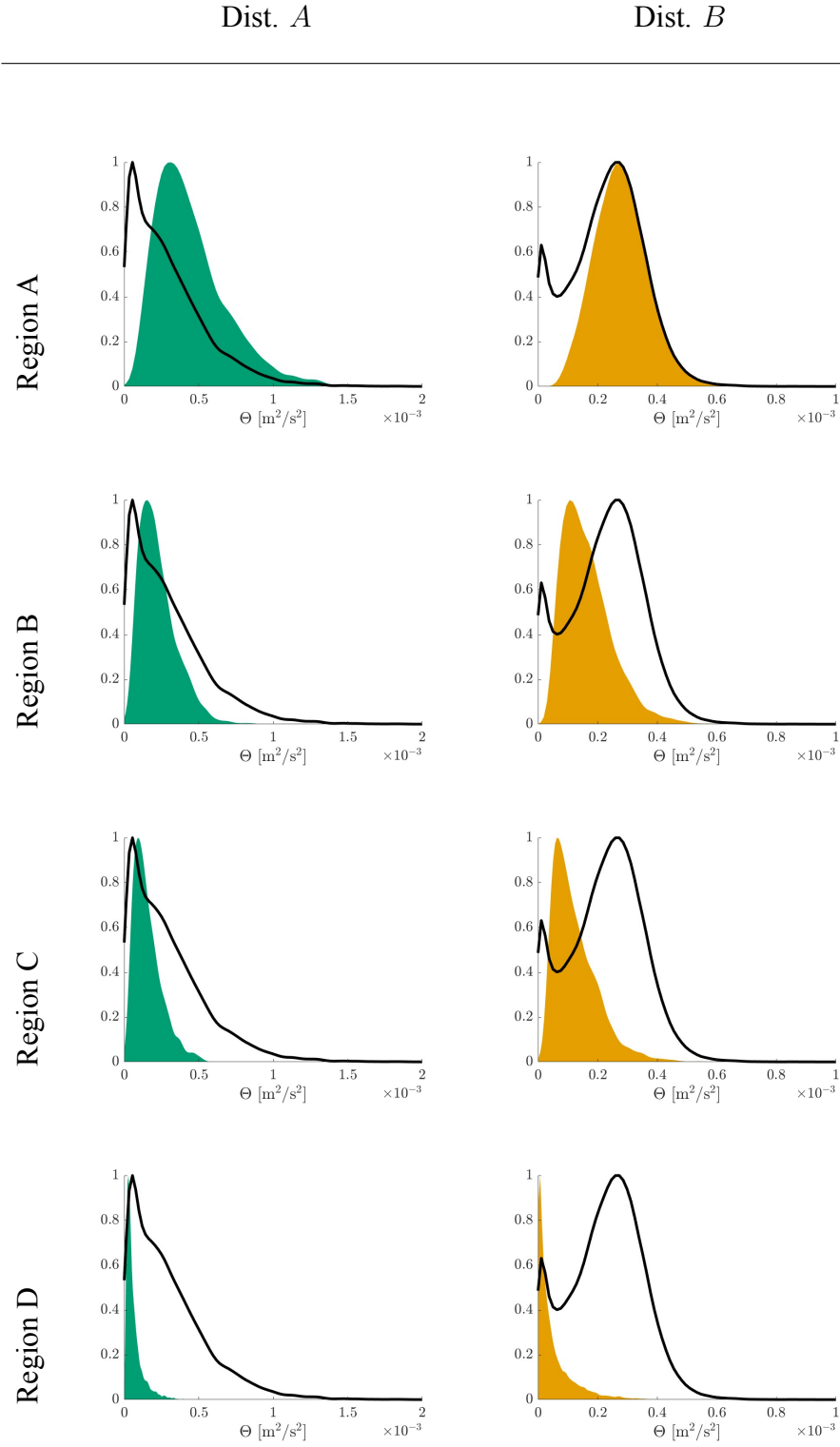


Figure 3.8: Summary of the granular temperature based on local volume fraction for the polydisperse distributions *A* (teal) and *B* (mustard) at $\langle \alpha_p \rangle = 0.01$.

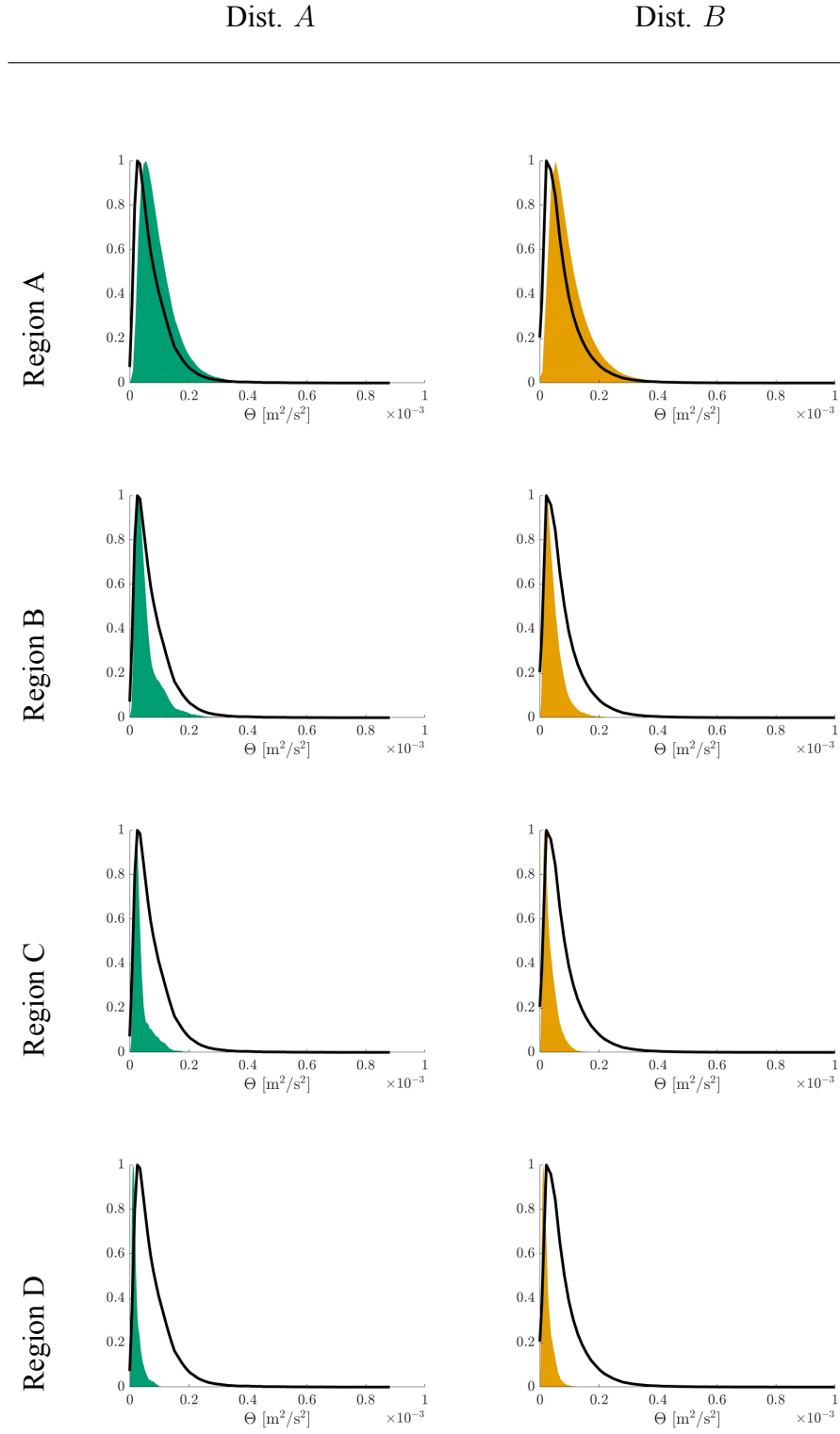


Figure 3.9: Summary of the granular temperature based on local volume fraction for the polydisperse distributions A (teal) and B (mustard) at $\langle \alpha_p \rangle = 0.10$.

3.3.2 STATISTICALLY STATIONARY ANALYSIS OF SETTLING BEHAVIOR

In this section, the settling behavior of each of the configurations under study, with a particular focus on how clustering behavior implicates settling, is examined. Existing predictions of settling velocity are discussed, followed by an analysis of settling behavior in clustering Regions A-D. Lastly, a comparison of existing settling predictions and simulated data is used to infer new settling model predictions.

To begin this analysis, the distributions of particle velocity and particle diameter in Regions A-D, in direct analogy with the discussion in the previous section, are considered. Figures 3.10-3.13 show these distributions, where the solid lines denote the distribution for the full domain and the shaded distributions denote the distribution for the given region of the flow. It is important to note that particle velocities in the cross-stream direction (v_p and w_p) are nearly equal, so only v_p is shown here.

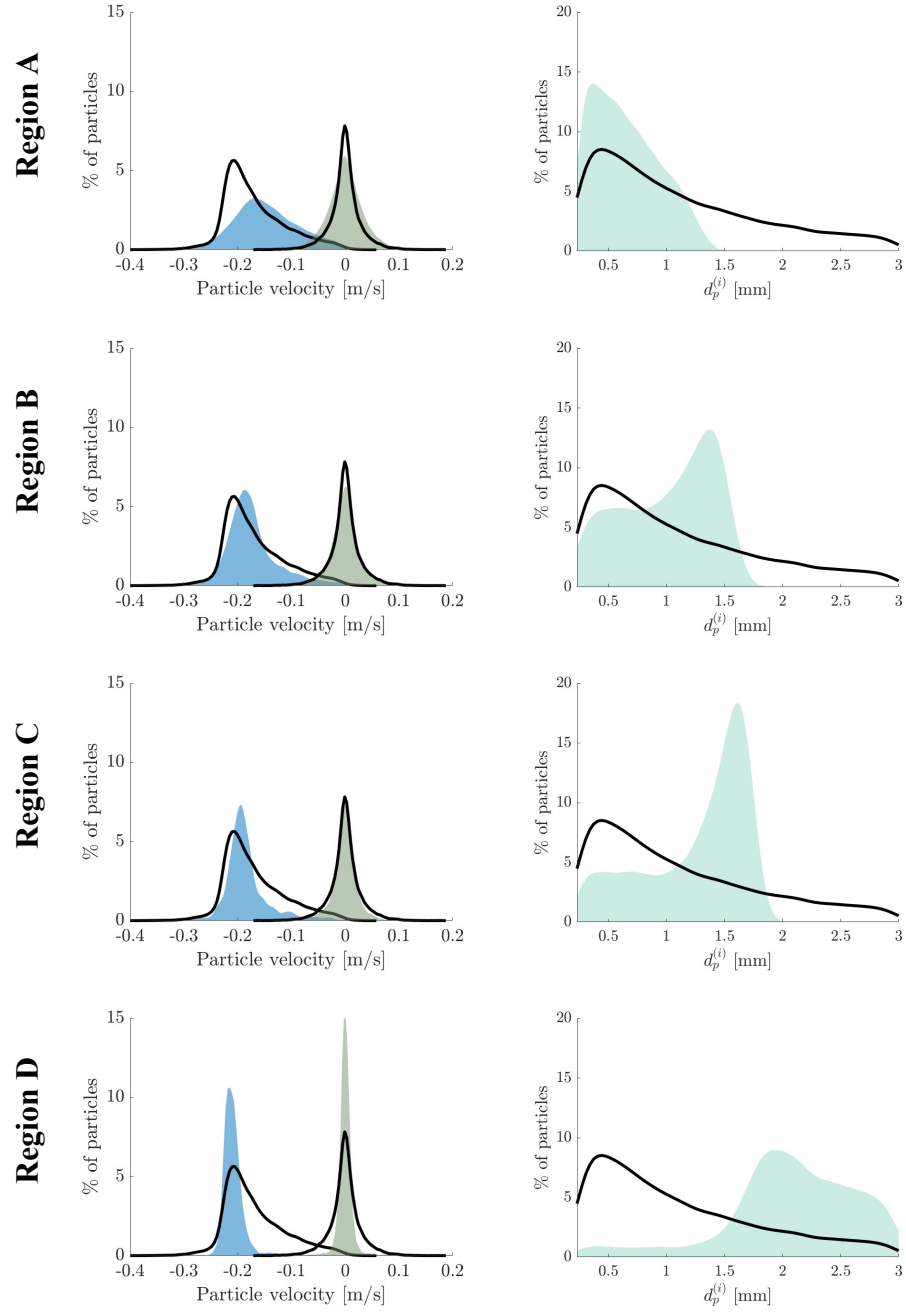


Figure 3.10: Distributions of particle velocities (u_p shown in blue and v_p shown in green) and distribution of particle diameter (shown in mint green on right) for Dist. A, $\langle \alpha_p \rangle = 0.01$. Distributions are shown for dilute to dense regions of the flow (top to bottom). The thick black line represents the total domain. Percent of particles in region A = 50.34 %, region B = 16.17 %, region C = 8.70 %, and region D = 24.80 %

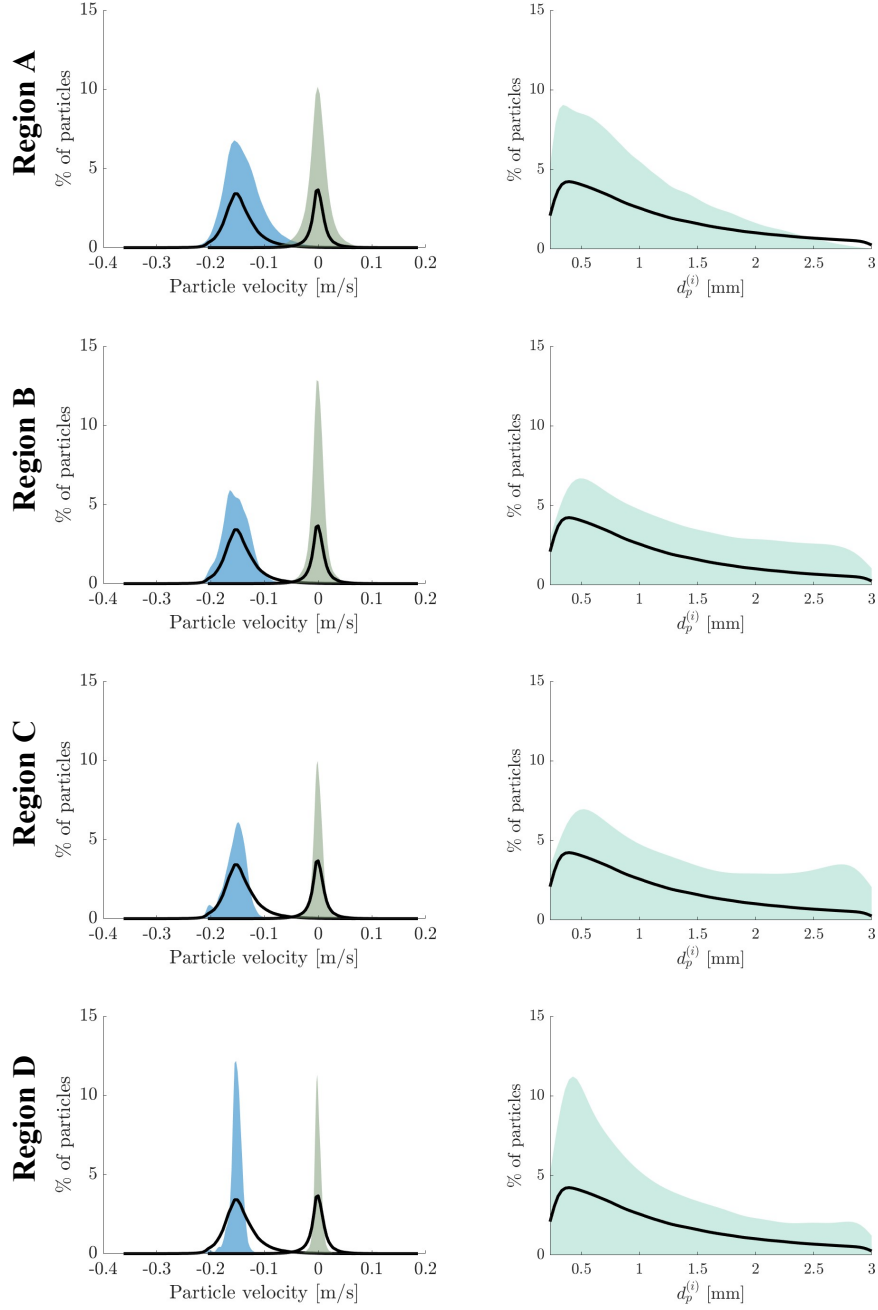


Figure 3.11: Distributions of particle velocities (u_p shown in blue and v_p shown in green) and distribution of particle diameter (shown in mint green on right) for Dist. A, $\langle \alpha_p \rangle = 0.10$. Distributions are shown for dilute to dense regions of the flow (top to bottom). The thick black line represents the total domain. Percent of particles in region A = 59.39 %, region B= 22.71 %, region C= 9.41 %, and region D= 8.48 %

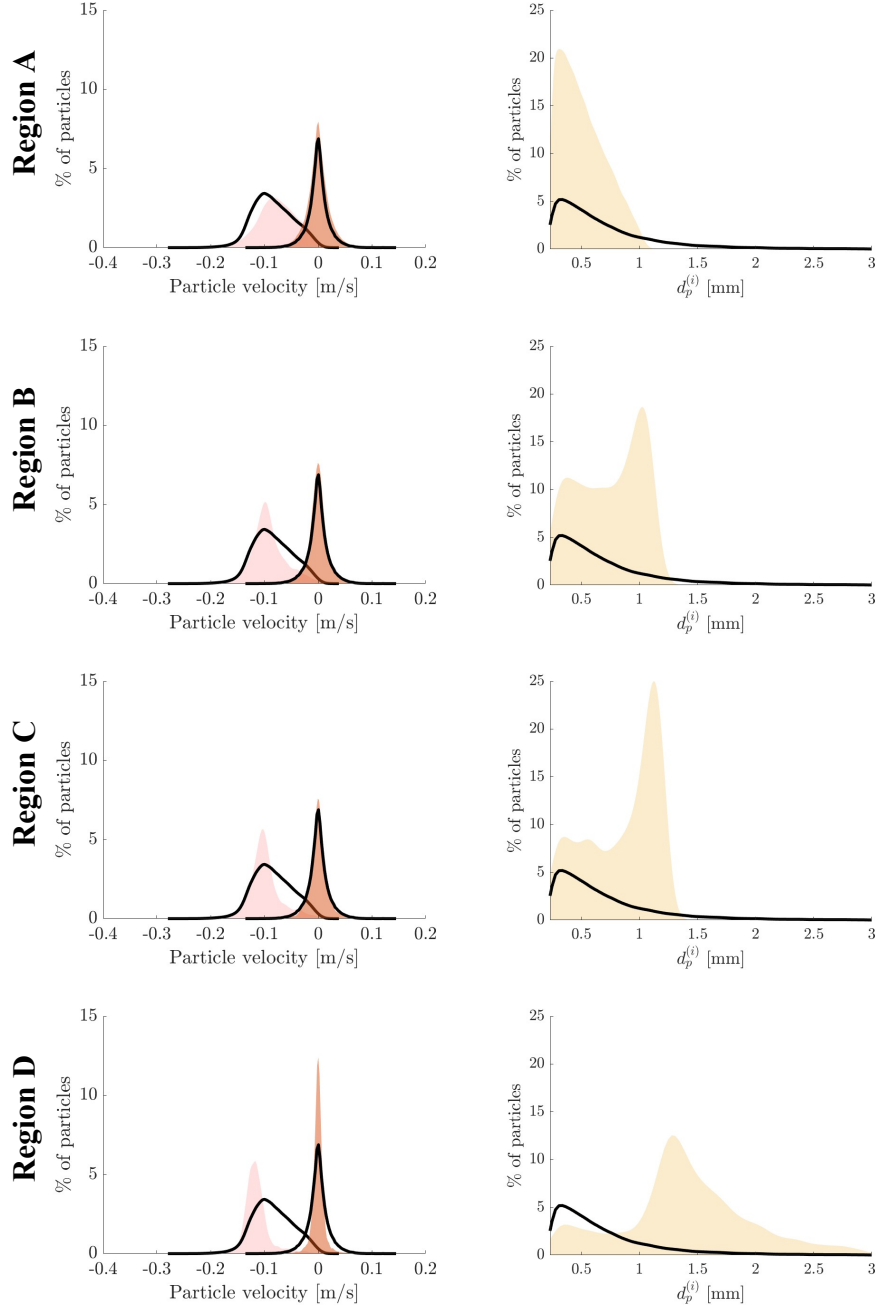


Figure 3.12: Distributions of particle velocities (u_p shown in pink and v_p shown in orange) and distribution of particle diameter (shown in yellow on the right) for Dist. B , $\langle \alpha_p \rangle = 0.01$. Distributions are shown for dilute to dense regions of the flow (top to bottom). The thick black line represents the total domain. Percent of particles in region A = 71.10 %, region B= 9.0 %, region C= 4.32 %, and region D= 15.60 %

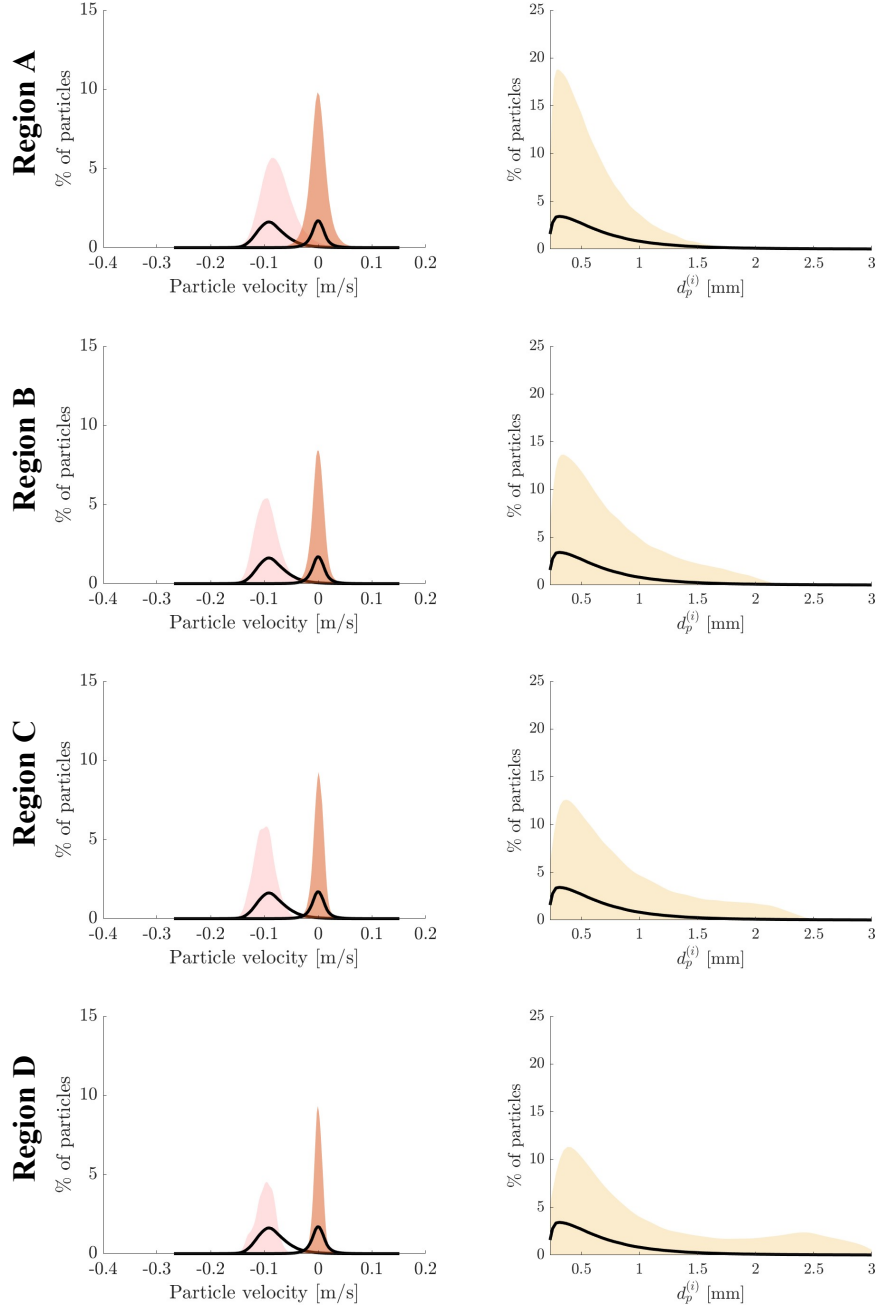


Figure 3.13: Distributions of particle velocities (u_p shown in pink and v_p shown in orange on the left) and distribution of particle diameter (shown in yellow on the right) for Dist. B , $\langle \alpha_p \rangle = 0.10$. Distributions are shown for dilute to dense regions of the flow (top to bottom). The thick black line represents the total domain. Percent of particles in region A = 62.96 %, region B= 19.10 %, region C= 10 %, and region D= 7.95 %

Smaller particles are more often located in Region A, with this effect being stronger when the volume fraction $\langle\alpha_p\rangle$ is 0.01. For these dilute cases, all particles in Region A are smaller than D_{30} , although this does not hold for higher volume fractions. It is observed that particles in Region A, the most dilute region, have statistically smaller streamwise settling velocities. This implies that particles are generally lone and have smaller settling velocities and occasionally velocities that oppose gravity. In the cross-stream directions (v_p and w_p), particles in Region A are more likely to attain larger velocities, indicating that they are more susceptible to being entrained in the underlying turbulence of the flow. This observation is consistent across all four polydispersed configurations. Distribution *A* and *B* at $\langle\alpha\rangle_p = 0.01$ contain a greater percentage of particles in the most dilute region (Region A), while Distribution *A* and *B* at $\langle\alpha\rangle_p = 0.10$ contain a greater percentage of particles in the most dense region (Region D). This can be due to the larger number of particles present in Distributions *A* and *B* at $\langle\alpha\rangle_p = 0.10$, causing an increase in the formation of correlated particles.

In Regions B and C, there is a dramatic increase in the probability of mid-sized particles for both Dist. *A* and *B*. Dist. *A* and *B* at high volume fraction exhibit a steady increase toward larger particles in Regions B and C, while the particle diameter for the dilute cases for Dist. *A* and *B* are more randomly distributed. Region C is most likely to contain larger particles at high volume fraction for both distributions.

Dist. *A* and *B* have a steady increase towards larger particles as the volume fraction rises; this trend continues through Region D. In Region D, very large particles are

also more common, though there's a noticeable drop in mid-sized particles. As cluster density grows, larger particles are more commonly found, while the presence of smaller particles decreases. This trend is particularly pronounced in Distribution *A*. As the particles form into dense clusters, they attain cross-stream velocities (v_p and w_p) near zero. This overall behavior is the same in both distributions *A* and *B* and at both mean volume fractions, however, Dist. *A* has a narrower band of cross-stream velocities in Region D compared with Dist. *B*, indicating that Dist. *A* clusters are more 'rigidly' packed, and particles are less able to move in the cross-stream directions.

This discussion highlights how particle behavior in each flow region depends on local volume fraction, but it's also useful to link settling behavior to particle size. In Section 3.3.1.3, it was shown that particle size affects clustering potential, so the relationship between particle size and settling velocity is tied to a particle's tendency to cluster.

At steady state, all the forces acting on the particles are in equilibrium. In particular, As described in Section 2.0.1.2, the drag force on a particle is given as

$$\mathbf{F}_{\text{drag}}^{(i)} = \frac{m_p^{(i)} \alpha_f [\mathbf{x}_p^{(i)}] F_d}{\tau_p} (\mathbf{u}_f [\mathbf{x}_p^{(i)}] - \mathbf{u}_p^{(i)}) . \quad (3.14)$$

Where F_d is the correction based on particle Reynolds number and local volume fraction [44]. As the drag force increases, particle settling velocity is hindered, and conversely, when the drag decreases, settling is enhanced. Drag force is complex and is a

function of many key quantities: local volume fraction, particle size, and slip velocity (see Eq. (2.8)). Careful consideration of these variables is taken into account when quantifying the effects of drag on particle settling.

To illustrate this behavior, Figures 3.14 and 3.15 show the relationship between individual particle settling velocities and drag forces against local volume fraction for six bins of particle size. Beginning with Figure 3.14, it is shown that the smallest particles achieve the widest range of settling velocities for all polydisperse configurations under study and that this occurs primarily in the dilute region of the flow. In denser regions of the flow, particle settling behavior becomes narrower, affecting primarily larger particles, indicating that particles have become more correlated with clusters. This is probably an intuitive result, as smaller particles are involved in jet bypassing phenomena and therefore are the only particles to attain a positive settling velocity (opposing gravitational direction).

Figure 3.15 shows the drag felt by each particle. The drag force increases with both volume fraction and particle diameter. In both volume fractions under study, Dist. *B* displays a narrower drag force. This implies that distributions with smaller mean diameters, even though containing more particles, experience less drag around the formed cluster. At high volume fraction, both distributions exhibit a wider range of drag experienced by each particle, due to larger clusters.

Figures 3.16 and 3.17 show the settling velocity against diameter for each particle in the simulation domain. A solid dark line represents the moving average of settling

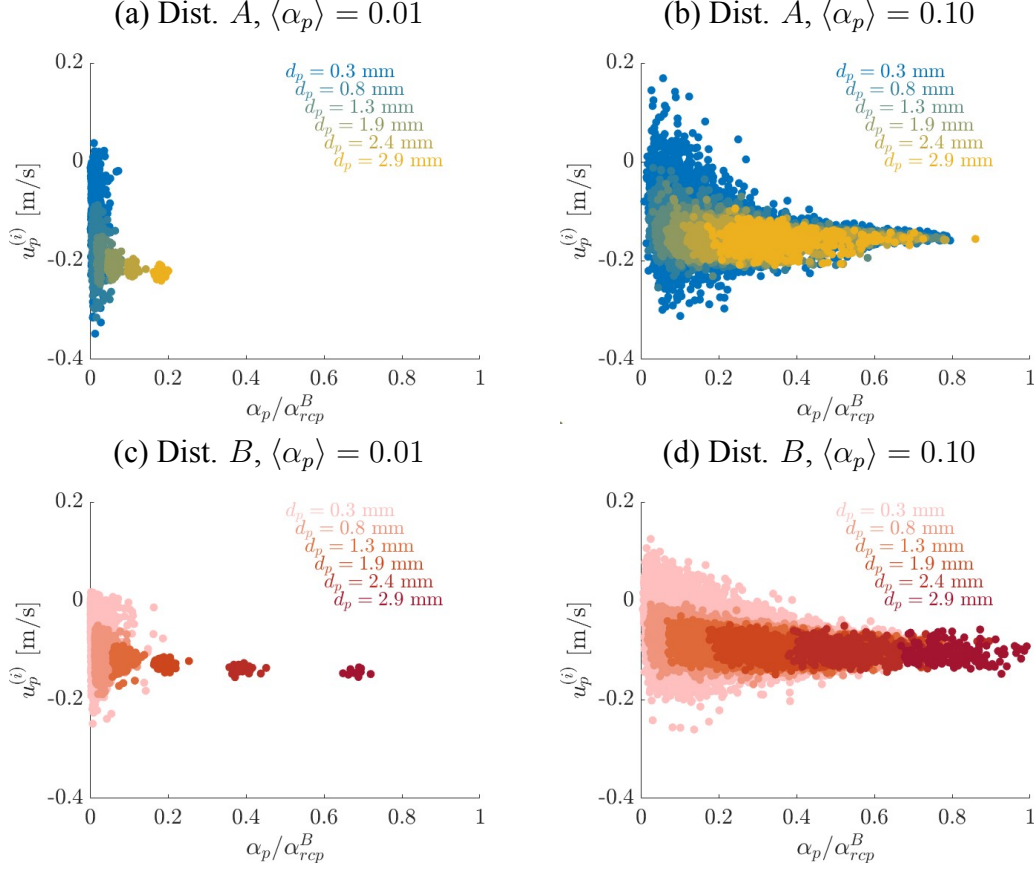


Figure 3.14: Settling velocity of individual particles plotted against normalized local particle volume fraction for all four polydisperse cases under consideration. Colors correspond to six increasing diameters $d_p = (0.3, 0.8, 1.3, 1.9, 2.4, 2.9)$ [mm] and the color maps for distributions A and B used throughout. The data plotted represents the particles within the diameters listed ± 0.03 mm.

velocity as a function of particle diameter. The results show that settling velocity increases with particle diameter, eventually approaching an asymptotic limit. This is consistent across all configurations under study. The data shows that smaller particles experience the widest range of settling velocities and are the only particles to attain a positive settling velocity, mirroring the trend seen in Figure 3.14. This phenomenon is observed across all four polydisperse configurations, suggesting that smaller particles can be influenced by the reduced drag wake created by larger leading particles. It is also observed that the

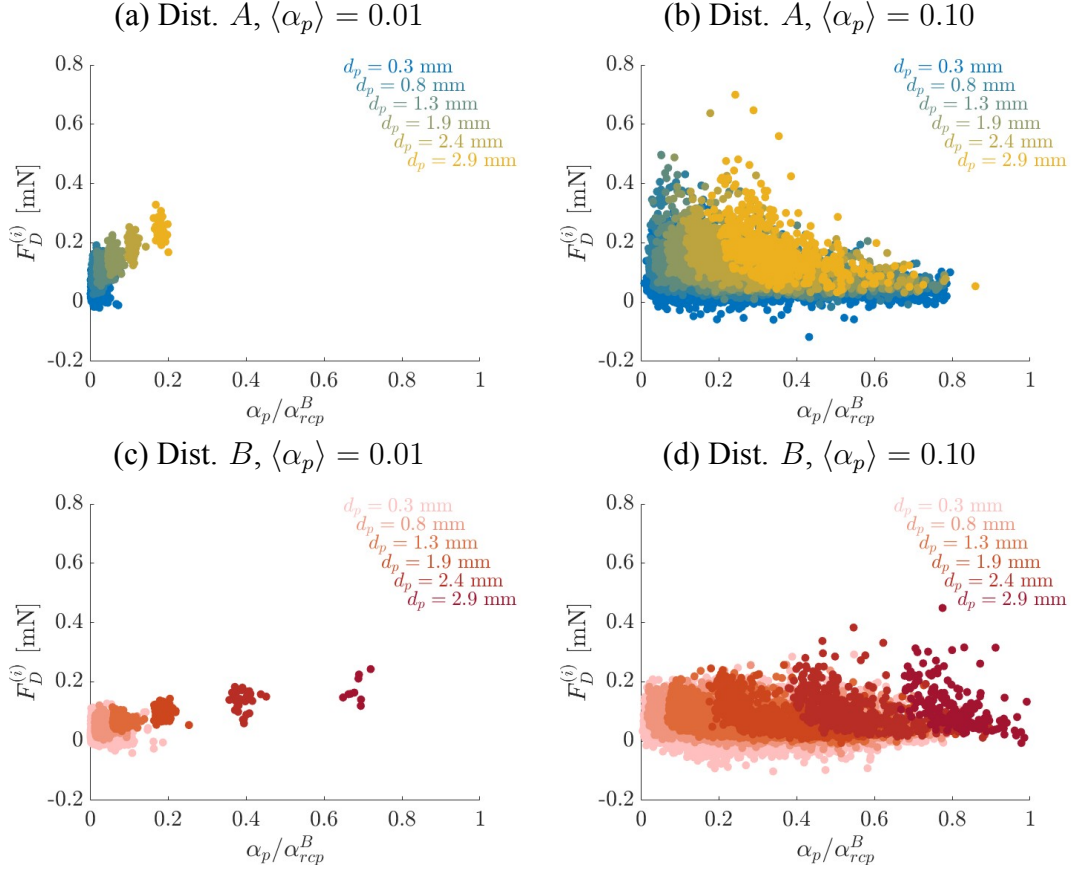
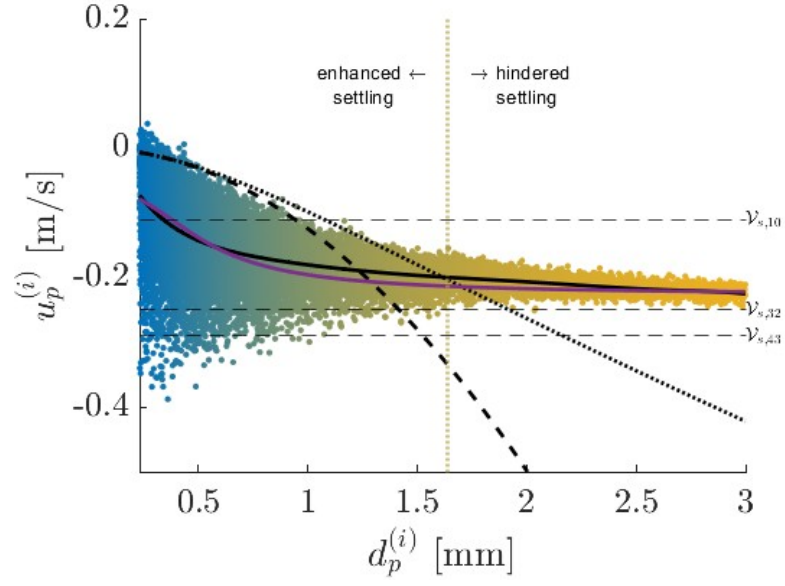
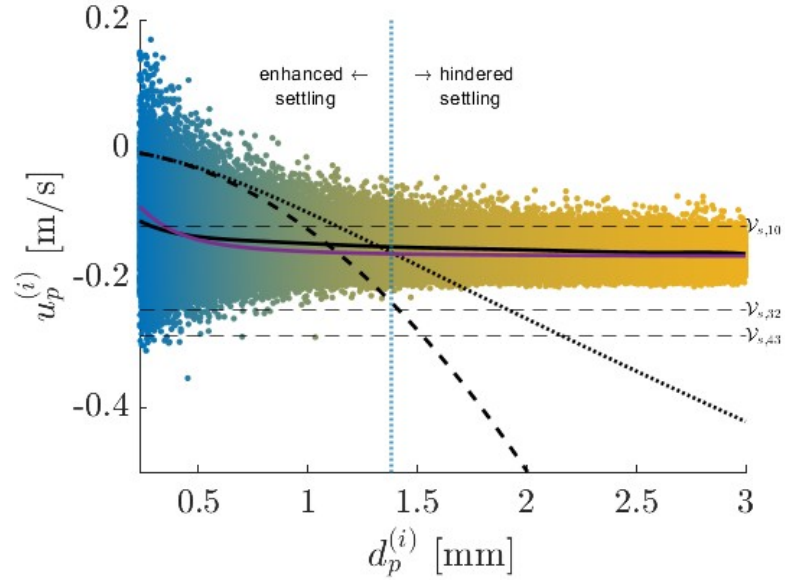


Figure 3.15: Drag force on individual particles plotted against normalized local particle volume fraction for all four polydisperse cases under consideration. Colors correspond to six increasing diameters $d_p = (0.3, 0.8, 1.3, 0.9, 2.4, 2.9)$, and the color maps for distributions A and B are used throughout. The data plotted represents the particles within the diameters listed ± 0.03 mm.

settling velocities are more varied for Dist. A compared with B . The spread of particle velocities for very fine particles is more widespread at $\langle\alpha_p\rangle = 0.10$.

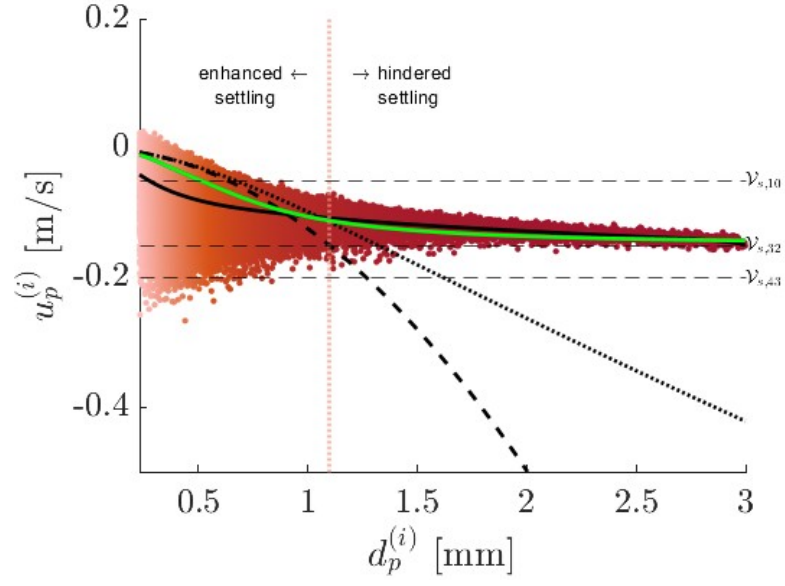


(a) $\langle \alpha_p \rangle = 0.01$, $d_p^{\text{crit}} = 1.64$ mm

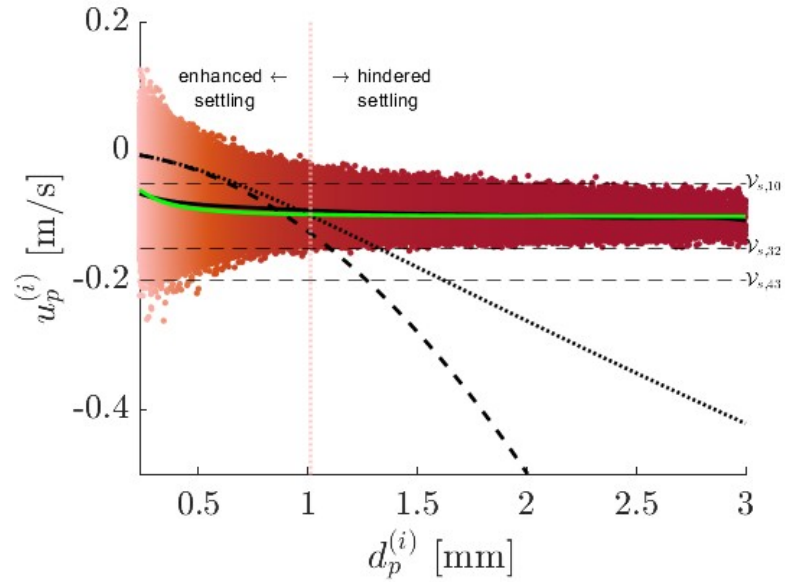


(b) $\langle \alpha_p \rangle = 0.10$, $d_p^{\text{crit}} = 1.38$ mm

Figure 3.16: Settling velocity as a function of particle diameter for Distribution A. Particles are colored by diameter (blue = small, yellow = large). The shaded background denotes the particle diameter PDF. The horizontal dashed lines represent the predicted settling velocities corresponding to D_{10} , D_{32} , and D_{43} using Eq. (3.15). The heavy solid line denotes the mean settling velocity as a function of particle diameter. The vertical line indicates the critical diameter, d_p^{crit} , separating enhanced settling for smaller particles and hindered settling for larger particles relative to Eq. (3.15). The loosely dashed line represents the prediction of the Stokes settling velocity, while the purple solid line is the proposed settling model given by Eqs. (3.17) and (3.18).



(a) $\langle \alpha_p \rangle = 0.01$, $d_p^{\text{crit}} = 1.10$ mm



(b) $\langle \alpha_p \rangle = 0.10$, $d_p^{\text{crit}} = 1.01$ mm

Figure 3.17: Settling velocity as a function of particle diameter for Distribution *B*. Particles are colored by diameter (pink = small, red = large). The shaded background denotes the particle diameter PDF. The horizontal dashed lines represent the predicted settling velocities corresponding to D_{10} , D_{32} , and D_{43} using Eq. (3.15). The heavy solid line denotes the mean settling velocity as a function of particle diameter. The vertical line indicates the critical diameter, d_p^{crit} , separating enhanced settling for smaller particles and hindered settling for larger particles relative to Eq. (3.15). The loosely dashed line represents the prediction of the Stokes settling velocity, while the green solid line is the proposed settling model given by Eqs. (3.17) and (3.18).

The Stokes settling velocity, $\mathcal{V}_0 = \tau_p g$ with $\tau_p = \rho_p d_p^2 / (18\mu_f)$ as previously defined, has traditionally been used to predict particle settling in multiphase flows [50–52], often in the absence of more sophisticated *a priori* predictors. Depth-averaged equations are commonly employed in volcanology to describe gravity-driven flows whose horizontal length scales greatly exceed their vertical length scales [91, 170, 199]. These models typically adopt an E-E framework to represent the dispersed phase and require a model for the particle settling velocity.

One commonly adopted approach is to compute the settling velocity using the Schiller-Naumann drag correlation [200], which was incorporated into multiphase flow models by Gidaspow [89]. The Schiller-Naumann model extends Stokes’ law by introducing a Reynolds-number-dependent drag coefficient to account for inertial effects at finite particle Reynolds numbers. The drag force is computed from the relative velocity between the particle and the surrounding fluid and assumes isolated, rigid, spherical particles settling in a dilute suspension. Consequently, the model neglects particle-particle interactions, hindered settling, particle clustering, and CIT. Under these assumptions, the depth-averaged settling velocity is given by

$$\mathcal{V}_s = \sqrt{\frac{4}{3C_D} g d_p \left(\frac{\rho_p - \rho_f}{\rho_f} \right)}, \quad (3.15)$$

$$C_D = \begin{cases} \frac{24}{\text{Re}} (1 + 0.15\text{Re}^{0.687}), & \text{Re} \leq 1000, \\ 0.44, & \text{Re} > 1000, \end{cases} \quad (3.16)$$

Table 3.5: Summary of the mean settling velocity for each configuration compared with Stokes' law and the settling law of [201] with several mean diameters used as input. Note that for monodisperse assemblies, the single value for each settling law is reported under the columns corresponding to the result using the d_{10} diameter as an argument. All velocities are shown in meters per second.

$\langle \alpha_p \rangle$	Dist.	$\langle u_p \rangle$	$\mathcal{V}_{0,10}$	$\mathcal{V}_{0,20}$	$\mathcal{V}_{0,32}$	$\mathcal{V}_{s,10}$	$\mathcal{V}_{s,20}$	$\mathcal{V}_{s,32}$
0.01	A_0	-0.20	-0.37	—	—	-0.21	—	—
	A	-0.17	-0.15	-0.21	-0.45	-0.11	-0.15	-0.24
	B_0	-0.05	-0.05	—	—	-0.04	—	—
	B	-0.08	-0.06	-0.08	-0.21	-0.05	-0.07	-0.14
0.10	A_0	-0.16	-0.37	—	—	-0.21	—	—
	A	-0.14	-0.15	-0.21	-0.45	-0.11	-0.15	-0.21
	B_0	-0.06	-0.05	—	—	-0.04	—	—
	B	-0.08	-0.06	-0.08	-0.21	-0.05	-0.07	-0.15

where C_D is the coefficient of drag. Because the Schiller-Naumann correlation is formulated for a single particle diameter, it does not account for polydispersity and therefore requires the selection of a representative mean particle diameter. For completeness, settling velocity predictions obtained using the statistical mean diameters (D_{10} , D_{20} , and D_{32}) are summarized in Table 3.5.

For the monodisperse assemblies studied, the depth-averaged settling velocity $\mathcal{V}_s$ predictor was more reliable when compared to Stokes settling. For the polydisperse configurations under study, using the surface mean diameter D_{20} as an input to Eq. (3.15) provided a more accurate approximation than that of the mean diameter D_{10} . As reported in Section 3.3.1.2, clustering and settling behavior are intimately connected and are more closely related to the surface mean diameter than the mean diameter.

Finally, a comparison is made between the steady-state data and existing settling predictions (Eq. (3.15)). As discussed earlier, $\mathcal{V}_{s,20}$ is reasonably predictive for *global*

mean settling behavior. It is important to note that both $\mathcal{V}_0$ and $\mathcal{V}_s$ fall short when predicting the settling behavior as a function of particle diameter. To illustrate this, Figures 3.16 and 3.17 show the predictions of both Stokes (loosely dashed line) and the model from de' Michieli Vitturi et al [201] (densely dashed line) as continuous functions of particle diameter.

Using Eq. (3.15) produces more accurate settling predictions in comparison to Stokes' assumption, but neither model approximates the mean settling behavior of particles over the range of diameters considered. The model Eq. (3.15) predicts an increasing settling velocity with diameter, approaching values much higher than observed for particles of similar size in the E-L data. This model does not account for cluster formation, which leads to the settling velocity reaching an asymptotic limit.

There is a critical particle diameter such that particles smaller than d_p^{crit} exhibit *enhanced* settling, and particles larger than d_p^{crit} exhibit *hindered* settling. This critical diameter denotes the intersection of the mean settling velocity and the depth-averaged prediction. These critical diameters are shown in Figures 3.16 and 3.17 as vertical dashed lines corresponding to the color of the particle diameter size. Smaller particles tend to settle faster than larger particles, which can be attributed to larger particles experiencing greater drag.

For both Distributions A and B , the critical diameter that separates enhanced from hindered settling is larger at $\langle \alpha_p \rangle = 0.01$ than at $\langle \alpha_p \rangle = 0.10$. At the higher volume fraction, the critical diameter is around d_{20} for Dist. A and d_{30} for Dist. B . At the lower

volume fraction, d_p^{crit} lies between d_{30} and d_{32} for both distributions. It is observed that denser distributions generally achieve higher average settling velocities, likely due to the greater number of particles present. Additionally, the range of settling velocities is narrower for the more dilute distributions.

In light of this data, an improved model is proposed in which the expression for the settling velocity, $\mathbb{V}_s$, retains the same functional expression as for $\mathcal{V}_s$,

$$\mathbb{V}_s^{(i)} = \sqrt{\frac{4}{3C_D} g d_p \left(\frac{\rho_p - \rho_f}{\rho_f} \right)} \quad (3.17)$$

but the expression for C_D is modified as

$$\begin{aligned} \mathbb{C}_D = \mathbb{M} \left[\frac{24}{\mathbb{NRe}_p} (0.2 + 0.01(\mathbb{NRe}_p)^{0.9}) + 0.35(\mathbb{NRe}_p) \right] - \frac{2}{(\mathbb{NRe}_p)^2 + 0.09} \\ + \frac{\mathbb{PW}}{1 + \mathbb{Re}_p^2}. \end{aligned} \quad (3.18)$$

where $\mathbb{M}$, $\mathbb{N}$, and $\mathbb{P}$ are constant coefficients summarized in Table 3.6.

Table 3.6: Summary of the model coefficients for the configurations studied.

$\langle \alpha_p \rangle$	Distribution	M	N	P
0.01	A_0	1.25	1.00	
	A	1.00	1.00	5.00
	B_0	14.00	1.00	
	B	3.50	1.00	5.00
0.10	A_0	1.25	3.00	
	A	1.00	2.50	0.10
	B_0	10.00	3.00	
	B	2.20	5.00	5.00

To quantify the improvement provided by the proposed drag model, the mean absolute error (MAE) and root-mean-square error (RMSE) were computed for both the proposed model and the original drag correlation using the mean as a reference point.

Across the four configurations, the proposed model reduced the RMSE relative to the original correlation by approximately 67%–88%. The reductions were 88.2% for Dist. A at $\langle \alpha_p \rangle = 0.01$, 81.4% for Dist. A at $\langle \alpha_p \rangle = 0.10$, 81.7% for Dist. B at $\langle \alpha_p \rangle = 0.01$, and 67.1% for Dist. B at $\langle \alpha_p \rangle = 0.10$. Averaged across all four cases, the proposed model produced an approximately 79.6% reduction in RMSE and a 76.2% reduction in MAE. These results demonstrate that the proposed model more accurately reproduces the Reynolds-number-dependent drag behavior observed in the particle-resolved simulations.

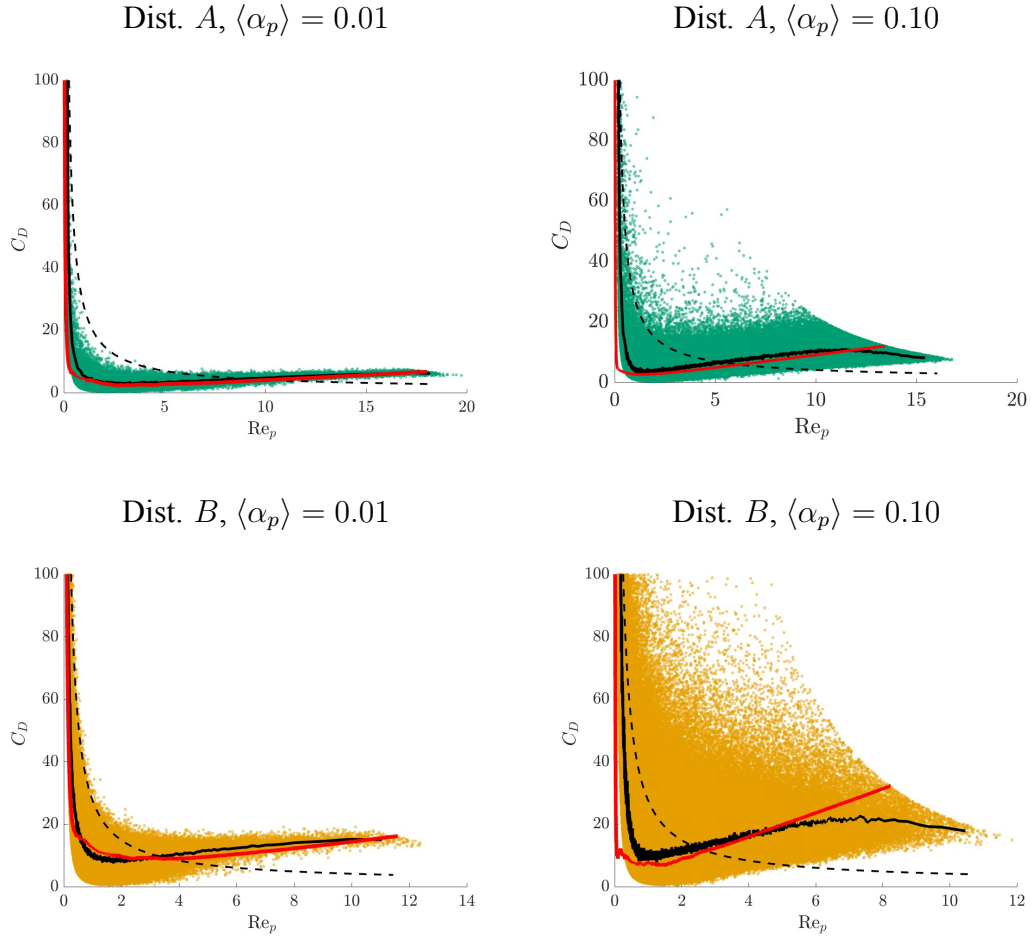


Figure 3.18: Coefficient of drag required to ensure $\mathbb{V}_s^{(i)} = u_p^{(i)}$, using the expression in Eq. (3.17). Values for individual particles are shown as shaded dots, the mean of this data as a function of particle diameter is shown as a dark black line, and the models for C_D are shown as dashed lines (black dashed is the baseline model of [201] and the red solid is the proposed new model shown in Eq. (3.17).

To begin, the coefficient of drag, C_D , required to result in the settling velocity observed in the highly resolved simulations was computed. For this portion of the study,

C_D takes the following form and is evaluated for each particle.

$$C_D = \frac{W}{0.5\rho_f V_o^2 \left(\pi \left(\frac{d_p}{2} \right)^2 \right)}, \quad (3.19)$$

where W is given as

$$W = \rho_p \mathcal{G} \frac{4}{3} \pi (d_p/2)^3, \quad (3.20)$$

and the particle Reynolds number is defined as,

$$\text{Re}_p = \frac{|\mathbf{u}_p| d_p}{\nu_f}. \quad (3.21)$$

These results are shown in Figure 3.18 for all particles in the configuration. The dark shaded line represents the mean of the data as a function of particle size. Overall, the proposed model, shown in red, provides a more accurate representation of the mean drag coefficient, with an exception for the dense Dist. *B* configuration at high Reynolds numbers. This deviation can be attributed to the larger amount of particles in the domain. Similar behavior is also observed in Dist. *A* at high volume fraction. Results for the monodispersed assemblies are summarized in Table 3.7.

Table 3.7: Predictions of the proposed model summarized alongside the mean settling velocity from the Euler-Lagrange studies and the Stokes prediction for the monodisperse assemblies.

$\langle \alpha_p \rangle$	Distribution	$\langle u_p \rangle$	$\mathcal{V}_0$	$\mathbb{V}_s$
0.01	A_0	-0.201	-0.367	-0.200
	B_0	-0.047	-0.050	-0.047
0.10	A_0	-0.146	-0.367	-0.144
	B_0	-0.056	-0.050	-0.056

The proposed drag model, Eq. (3.18), was developed by modifying the correlation of de' Michieli Vitturi et al. [201] based on the relationship between the computed drag coefficient and particle Reynolds number obtained from the highly resolved simulation data. The first term represents a modified Schiller-Naumann correlation that preserves the transition between the viscous and inertial drag regimes while improving agreement with the simulation data. The second term accounts for hindered settling, which becomes increasingly important for larger particles and denser suspensions. The third term represents the enhanced settling observed for smaller particles due to particle-fluid interactions that are not captured by classical drag correlations. Finally, the fourth term introduces stochastic fluctuations in drag through a Wiener process, $\mathcal{W}$, to account for the random variability arising from particle clustering and the inherently unsteady nature of the flow. The Wiener process is implemented numerically as illustrated in Figure 3.19,

while the relative contribution of each term to the total drag coefficient for Distribution A is shown in Figure 3.20.

```
T = max(Rep); dt = T/Npart;

dW = zeros(1,Npart);

W = zeros(1,Npart);

dW(1) = sqrt(dt)*randn;

W(1) = dW(1);

for j = 2:Npart

    dW(j) = sqrt(dt)*randn;

    W(j) = W(j-1) + dW(j);

end
```

Figure 3.19: Summary of the numerical implementation of the Wiener process. This code snippet is written in the style of MATLAB, where ‘randn’ represents a normally distributed random number bounded by $[0, 1]$.

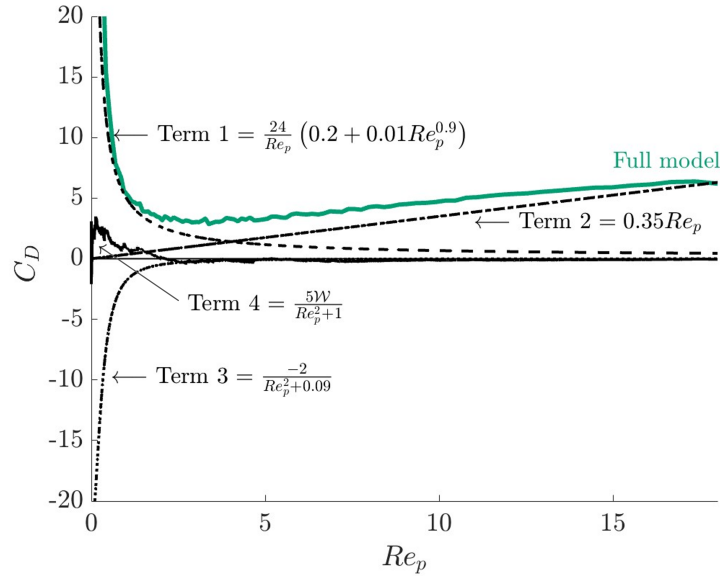


Figure 3.20: Exemplary case (Dist. A, $\langle \alpha_p \rangle = 0.01$) demonstrating the relative contribution of each of the terms in the proposed coefficient of drag model in Eq. (3.17).

The coefficients $\mathbb{M}$, $\mathbb{N}$, and $\mathbb{P}$ were determined using ordinary least-squares (OLS) regression by fitting Eq. (3.18) to the simulation data. Consequently, the proposed relationship should be interpreted as a semi-empirical drag correlation that is valid over the range of particle Reynolds numbers, particle size distributions, and particle volume fractions considered in this study. Its applicability outside this parameter space has not been established and requires additional validation. In particular, it is postulated that $\mathbb{M} = f(\sigma, \mu, d_{10}, d_{20}, d_{30}, d_{32}, d_{43})$ and $\mathbb{N} = f(\langle \alpha_p \rangle)$.

3.4 CONCLUSIONS

In this work, the effects of polydispersity on particle clustering and settling behavior using highly resolved Euler-Lagrangian simulations of two polydisperse particle distributions and two analogous monodisperse particle distributions were analyzed. These four particle

distributions were studied at two volume fractions ($\langle\alpha_p\rangle = 0.01$ and $\langle\alpha_p\rangle = 0.10$), and all simulation parameters were sampled to align with values typical of PDCs.

When particles interact strongly with each other and are influenced by gravity, clusters naturally form, affecting how particles settle compared to when they are evenly dispersed. However, the role of polydispersity in shaping these clusters and influencing settling behavior has not been well understood.

This study shows that mass loading, a common measure used to predict clustering, is inadequate, especially for mixtures of different particle sizes. This is because mass loading does not account for the distribution of mass within the system. Instead, *surface loading*, a new measure based on the average surface diameter of particles, was introduced. Surface loading better predicts clustering and settling behavior, leading to two new models developed in this work.

This work identifies the surface mean diameter, D_{20} , as the most effective choice for predicting mean flow behavior using models like the settling velocity model from [201]. While D_{20} improves predictions for average settling, existing models still fail to capture settling behavior across a range of particle sizes. Additionally, current models incorrectly predict that settling velocity keeps increasing with particle size. Instead, the settling velocity rises initially but then levels off due to the effects of clustering in the flow.

To address this, a new drag coefficient model that accurately predicts settling velocities for different particle sizes was proposed. This model is intended to be implemented in existing solvers, such as those in [201].

CHAPTER 4

THE EFFECT OF DOMAIN SIZE ON FLUID-PARTICLE STATISTICS IN POLYDISPERSE MULTIPHASE GAS-SOLID FLOWS

4.1 INTRODUCTION

The study of computational domain scaling is essential in particle-laden multiphase flows because the computational domain directly influences the development of CIT and the statistical quantities used to construct reduced-order models. Smaller domains can introduce artificial periodic effects and limit the development of flow structures, resulting in biased estimates of settling velocity, particle concentration fluctuations, turbulent kinetic energy, and other statistical quantities. Because these statistics are commonly used to develop *a priori* predictors and closure relationships for coarse-grained multiphase flow models, inadequate domain sizes can lead to closure models that are not representative of the underlying physics. Conversely, larger computational domains reduce artificial periodicity and improve statistical independence by allowing particle clusters and turbulent structures to evolve naturally. However, increasing the domain size also increases the number of particles, computational cells, and simulation time required to obtain statistically converged results. Determining an appropriate domain size therefore represents an important balance between computational efficiency and statistical accuracy.

Numerous numerical studies have demonstrated that velocity fluctuations in initially uniform, randomly distributed particle suspensions depend on the computational

domain size [202–206]. In contrast, early experimental studies [207–210] generally reported little or no domain-size dependence. This apparent discrepancy was later resolved by Segre et al. [211], who showed that velocity fluctuations scale with system size only when the computational domain is smaller than the characteristic correlation length, approximately twenty particle spacings. Once the domain exceeds this correlation length, both numerical and experimental studies exhibit good agreement, indicating that the resulting statistics are independent of domain size.

Capecelatro et al. [79] previously investigated the influence of computational domain size on fluid-particle statistics for *monodisperse* particle suspensions and established domain dimensions sufficient to obtain statistically converged settling and clustering behavior. That work serves as the foundation for the present study. This prior work studied assemblies of moderate-sized particles ($90\ \mu\text{m}$). However, extending these concepts to *polydisperse* systems is not straightforward. In monodisperse suspensions, the characteristic cluster length and computational domain can be scaled using a single particle diameter. In contrast, polydisperse systems contain a broad spectrum of particle sizes, each possessing different response times, settling velocities, and characteristic clustering behavior. Consequently, it is not immediately apparent which particle diameter should be used to define the characteristic cluster length or computational domain size. This uncertainty raises an important question for coarse-grained multiphase modeling: can a single domain scaling methodology accurately represent the statistics of a highly polydisperse suspension?

To address this question, this study investigates the influence of computational domain size on steady-state fluid-particle statistics in fully developed CIT for polydisperse particle suspensions ranging from $27\text{ }\mu\text{m}$ to 3 mm in diameter. The resulting analysis establishes domain scaling relationships for polydisperse systems and provides guidance for selecting computational domains that produce statistically converged settling, clustering, and turbulence statistics. These relationships are intended to improve the development of *a priori* predictors and closure models for coarse-grained multiphase flow solvers.

4.1.1 SYSTEM DESCRIPTION

This study considers three computational domain sizes, denoted by $L_1 \times L_2 \times L_3$, to investigate the influence of domain size on steady-state fluid-particle statistics in fully developed cluster-induced turbulence. The domain dimensions range from $1.44\mathcal{L} \times 0.18\mathcal{L} \times 0.18\mathcal{L}$ to $2.87\mathcal{L} \times 0.35\mathcal{L} \times 0.35\mathcal{L}$, thereby spanning domains smaller than and comparable to those previously shown to produce statistically converged results in monodisperse systems [79]. To isolate the effects of domain size, only a single polydisperse configuration, Distribution B (from the study in Chapter 3) at the high volume fraction, is considered. This configuration was selected because it exhibits the strongest clustering and therefore represents the most demanding case for assessing domain-size effects.

Table 4.1: Summary of configurations under study and relevant characteristic cluster lengths and response times.

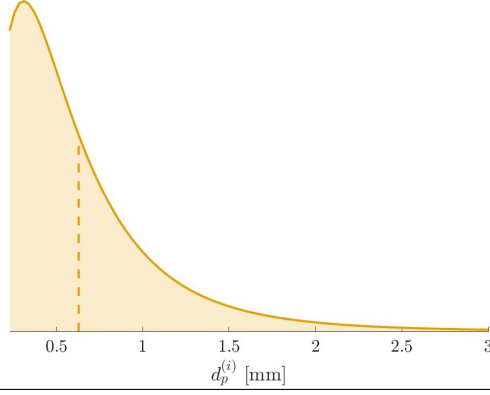
	<i>Configuration</i>		
	1	2	3
L_x [mm]	300	400	600
$L_{y,z}$ [mm]	37.5	50.0	75.0
N_x	746	994	1,492
$N_{y,z}$	94	126	188
N_p	92,497	219,923	745,037

All computational domains maintain a constant aspect ratio of 1 : 8, while the dimensions in each direction are increased proportionally so that changes in the measured statistics can be attributed solely to the overall domain size rather than the domain geometry. The grid spacing is held constant at $\Delta x = 1.75 d_{p,\min}$, resulting in progressively larger uniform meshes as the domain size increases. Owing to the substantial computational expense associated with E-L simulations, larger computational domains require significantly more particles and grid cells to maintain the same spatial resolution. Consequently, the largest domain considered in this study, $2.87\mathcal{L} \times 0.35\mathcal{L} \times 0.35\mathcal{L}$, represents the largest computationally feasible configuration and contains $N_p = 745,037$ particles, whereas the smallest domain contains $N_p = 92,497$ particles. The physical parameters corresponding to each simulation are summarized in Table 4.2, while the domain dimensions are listed in Table 4.1.

To place the present study in the context with earlier work [79], the domain sizes associated with Configurations 1–3 lie within the range defined by Cases 4–6 in the referenced study, which employed gravity-aligned grids of $N_x = 512, 1024$, and 2048 ,

respectively. In prior work [79] a grid spacing of $\Delta x = 1.75 d_{p,10}$ was utilized. In this study, $\Delta x = 1.75 d_{p,min}$ in order to create a closer one-to-one comparison, given that $d_{p,10}$ in [79] is significantly smaller than the mean particle diameter in this study. In terms of particle count, the number of particles in Configurations 1–3 considered here falls between those reported for Cases 3 and 4 in the earlier work—specifically, 107,329 and 858,629 particles, respectively [79].

Table 4.2: Summary of simulation parameters under consideration. The PDF shown above the table represents the distribution from which particles were sampled and is specified according to log-normal parameters μ and σ . The dashed line represents the arithmetic mean particle diameter, d_{10} .



Particle-phase properties			
log-normal parameters	μ		-0.69
	σ		0.69
skewness	$\text{skew}(d_p)$		1.8
kurtosis	$\text{kurt}(d_p)$		7.1
cutoff diameters	$d_{\min}$	[mm]	0.23
	$d_{\max}$	[mm]	3.00
standard deviation	$\sqrt{\langle d_p'^2 \rangle}$	[mm]	0.43
arithmetic mean diameter	$d_{p,10}$	[mm]	0.69
surface mean diameter	$d_{p,20}$	[mm]	0.81
volume mean diameter	$d_{p,30}$	[mm]	0.95
surface moment mean diameter	$d_{p,32}$	[mm]	1.31
volume moment mean diameter	$d_{p,43}$	[mm]	1.65
particle relaxation times	$\tau_{p,10}$	[s]	3.57
	$\tau_{p,20}$	[s]	4.23
	$\tau_{p,30}$	[s]	6.77
	$\tau_{p,32}$	[s]	12.88
	$\tau_{p,43}$	[s]	20.44
Characteristic lengths	$\mathcal{L}_{\min}$	[mm]	2.50
	$\mathcal{L}_{0,10}$	[mm]	204.4
	$\mathcal{L}_{0,20}$	[mm]	388.2
	$\mathcal{L}_{0,30}$	[mm]	734.5
	$\mathcal{L}_{0,32}$	[mm]	2655.8
	$\mathcal{L}_{0,43}$	[mm]	6684.2
	$\mathcal{L}_{\max}$	[mm]	73046.0
Stokes settling velocities	$\mathcal{V}_{\min}$	[m/s]	-0.006
	$\mathcal{V}_{0,10}$	[m/s]	-0.057
	$\mathcal{V}_{0,20}$	[m/s]	-0.079
	$\mathcal{V}_{0,30}$	[m/s]	-0.108
	$\mathcal{V}_{0,32}$	[m/s]	-0.206
	$\mathcal{V}_{0,43}$	[m/s]	-0.327
	$\mathcal{V}_{0,\max}$	[m/s]	-1.081
Distribution-independent properties			
fluid density	ρ_f	[kg/m ³]	0.5
fluid viscosity	μ_f	[kg/(m s)]	1.85×10^{-5}
particle density	ρ_p	[kg/m ³]	2500
gravity	$\mathbf{g}$	[m/s ²]	(-0.016, 0, 0)
mass loading	φ		552.7
volume fraction	$\langle \alpha_p \rangle$		0.10

4.2 RESULTS

In this section, the observed clustering and settling behavior of the configurations under study are examined.

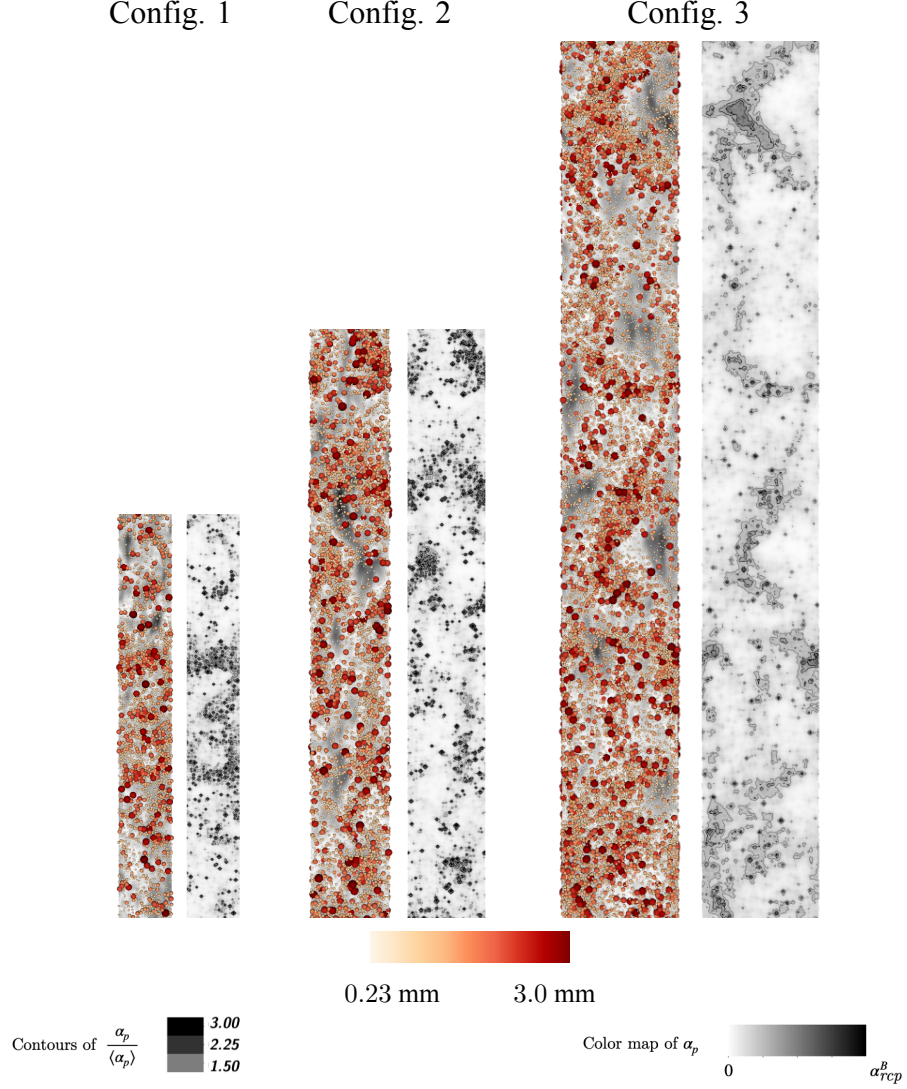


Figure 4.1: Representative snapshots from the statistically stationary period of each configuration under study. Each slice is an x - y plane at $z = 0$. On the leftmost snapshot for each configuration, fluid-phase velocity (gray) is normalized with the polydisperse Stokes settling velocity, $\mathcal{V}_{0,10}$, and particles are colored by diameter from pink (small) to red (large). On the rightmost snapshot for each configuration, there is a colormap for local volume fraction, wherein α_p ranges from 0 (white) to $\alpha_{rcp}^B = 0.7036$ (black) [78]. Also plotted are the corresponding contours denoting volume fractions of $(1.5, 2.25, 3.0)\langle \alpha_p \rangle$.

4.2.1 PARTICLE CLUSTERING BEHAVIOR

This section analyzes the clustering behavior observed in each configuration. The particle field's local volume fraction colormap is shown in Figure 4.1. Here, the color map is also overlaid with contours for regions that are 1.5, 2.25, and 3 times the mean volume fraction. The differences in clustering behavior across the configurations studied are minimal.

The degree of clustering, $\mathcal{D}$, detailed in Eq. (3.3), was calculated for each domain size under study to bolster these observations. The degree of clustering was 1.29, 1.18, and 1.20 for configurations 1, 2, and 3, respectively.

Because the configurations examined in this study most closely correspond to Cases 3–4 in Capecelatro et al. [79], where clustering behavior was observed to plateau, this suggests that the present studied domain sizes may be approaching the threshold required to capture CIT accurately. Additionally, the clustering intensity observed here is significantly greater than that reported for the monodisperse systems in Capecelatro et al. [79]. This outcome is consistent with trends identified in earlier work [78], where polydisperse particle systems exhibited enhanced clustering relative to their monodisperse counterparts. This behavior can be attributed to the influence of larger particles, which more strongly perturb the surrounding fluid and promote the entrainment of smaller particles in their wakes.

4.2.2 PARTICLE SETTLING BEHAVIOR

This section examines the settling behavior of each of the configurations under study, with a focus on how clustering behavior implicates settling behavior.

In the case of a monodisperse arrangement of particles, the PA scaling for the settling velocity relies on the mean particle diameter. With polydisperse configurations, other statistical diameters can be leveraged. Figure 4.2 (a) presents the scaling behavior of the cases considered in this study using four statistical particle diameters: the number mean diameter $d_{p,10}$, the surface-weighted diameter $d_{p,20}$, the volume-weighted diameter $d_{p,30}$, and the Sauter mean diameter $d_{p,32}$. Each scaling is represented using distinct markers and compared against the particle-averaged (PA) settling data and corresponding trends reported by Capecelatro et al. [79]. Notably, the present results, particularly those normalized by the larger characteristic diameters, show strong agreement with the overall trends identified in the prior study. Here $\mathcal{V}$ denotes the settling velocity of an isolated particle in undisturbed flow.

It is important to recognize that multiple characteristic particle diameters may serve as appropriate scaling parameters. As noted previously, the domain extents and particle counts considered in this study are comparable to those associated with Cases 3-5 in Capecelatro et al. [79]. To further examine this, Figure 4.2 (b) expands the analysis to include a broader spectrum of diameter-based scalings, spanning from the minimum particle size $d_{p,\min}$ (indicated by blue markers) to the maximum size $d_{p,\max}$.

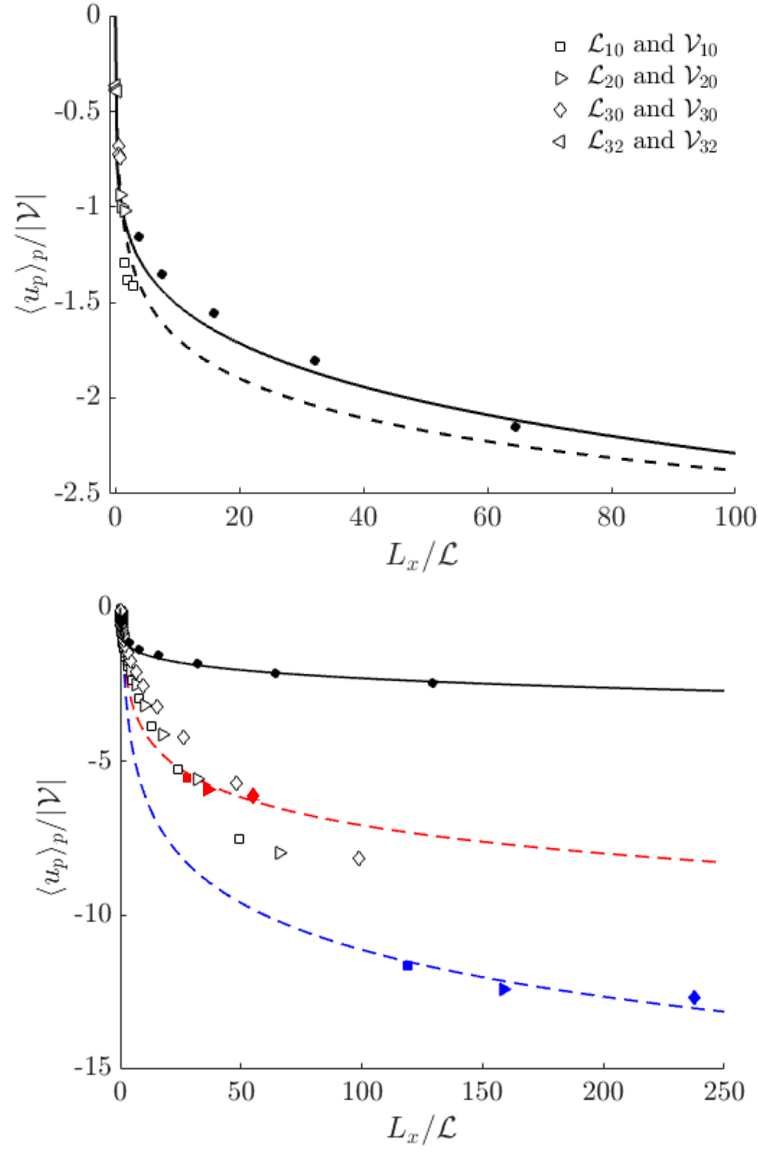


Figure 4.2: (a) The three cases studied in this work are scaled by standard statistical diameters as shown. A dashed curve of the form $\ln((L_x/\mathcal{L})^{-0.3}) - 1$ describes the scaling trend for data normalized according to $d_{p,10}$. The solid curve is that of Capecelatro et al. [79], $-(L_x/\mathcal{L})^{0.18}$, and solid square markers denote mean particle settling of the configurations studied in [79]. (b) Emphasis of the effect of scaling on settling behavior. Configurations 1, 2, and 3 are denoted by open squares, right-facing triangles, and diamonds, respectively. Each set of data is scaled continuously by a particle diameter bound by $d_{p,min}$ and $d_{p,max}$. Exemplary curves modeling this behavior are shown in red (scaling according to $d_{p,mode}$) and blue dashed lines (scaling according to $d_{p,min}$) along with their corresponding solid markers for each configuration.

A particularly informative result emerges when the mode of the particle size distribution is used as the characteristic length scale, defined as $d_{p,\text{mode}} = \exp(\sigma - \mu^2)$, where σ and μ are the log-normal distribution parameters listed in Table 4.2. Under this scaling, the normalized domain sizes align closely with Cases 3–5 from Capecelatro et al. [79]. These results, shown with red markers in Figure 4.2 (b), further highlight the increased settling rates observed in polydisperse systems relative to monodisperse ones.

To capture the observed trends, dashed curves (red and blue) are included to represent the relationship between normalized settling velocity and domain size. The power-law formulation proposed by Capecelatro et al. [79], $\langle u_p \rangle_p / |\mathcal{V}| = (L_x / \mathcal{L})^A$, where A is a constant, does not adequately describe the curvature of the present polydisperse data. In particular, the normalized settling velocity initially increases rapidly with domain size due to clustering, but the rate of increase slows as the system approaches a fully developed state.

To better represent the observed dependence of the normalized mean settling velocity on the ratio of the computational domain size to the characteristic particle spacing, a logarithmic relationship is proposed

$$\frac{\langle u_p \rangle}{\mathcal{V}} = \ln \left[\left(\frac{L_x}{\mathcal{L}} \right)^B \right], \quad (4.1)$$

where B is a constant determined using ordinary least-squares (OLS) regression.

For the scaling based on $d_{p,\text{mode}}$ (red dashed curve), $B = -1.32$, while for the $d_{p,\text{max}}$

scaling (blue dashed curve), $B = -2.2$. The logarithmic functional form was selected because the simulation results exhibit a rapid variation in normalized settling velocity at small values of $L_x/\mathcal{L}$, followed by a progressively weaker dependence as the domain size increases. A logarithmic relationship naturally captures this diminishing sensitivity while remaining monotonic over the range of the available data.

Furthermore, the proposed relationship satisfies the expected limiting behavior. As the computational domain approaches the characteristic particle spacing,

$$\lim_{L_x/\mathcal{L} \rightarrow 1} \ln \left[\left(\frac{L_x}{\mathcal{L}} \right)^B \right] = 0, \quad (4.2)$$

such that the normalized settling velocity approaches zero. This behavior is consistent with the expectation that cluster-induced settling enhancement vanishes as the computational domain becomes too small to support the formation of particle clusters. Although the logarithmic scaling was motivated by the observed trends in the simulation data and the expected asymptotic limit, the coefficient B was determined empirically using OLS regression. Consequently, the proposed relationship should be interpreted as a semi-empirical correlation that is valid over the range of domain sizes investigated in this study.

4.2.3 PARTICLE-PHASE AND FLUID-PHASE FLUCTUATING ENERGY BEHAVIOR

Lastly, the effects of domain scaling on steady-state two-point statistics, specifically on the fluctuating granular and turbulent kinetic energy are analyzed.

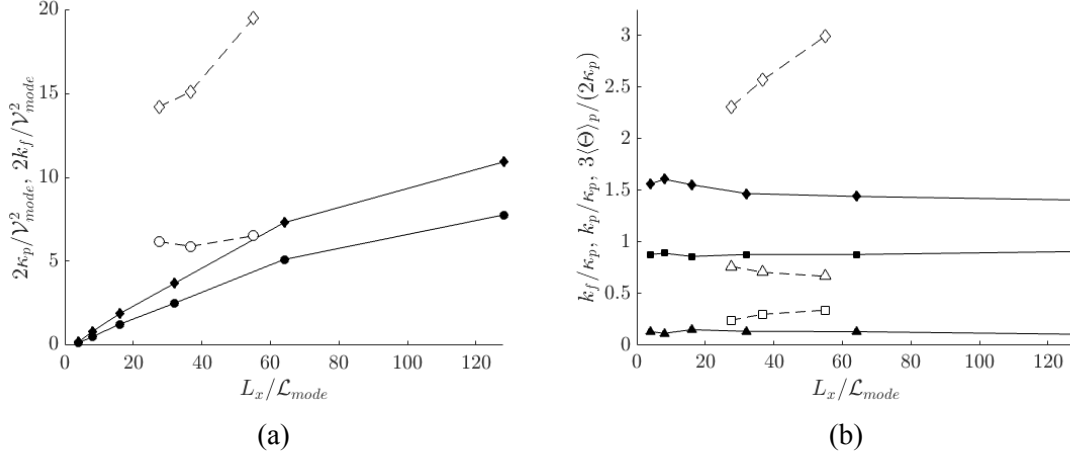


Figure 4.3: Fluctuating energy as a function of domain size. κ_p (circles), k_f (diamonds), k_p (squares), and Θ (triangles). Empty symbols and dashed lines represent the data from this work and filled symbols and solid lines are reproduced from Capecelatro et al. [79] for comparison (a) Total fluctuating energy of each phase normalized by $\mathcal{V}_{mode}^2$ and (b) separate contributions to the total particle-phase fluctuating energy normalized by κ_p .

The analysis begins by examining the total granular energy and fluid turbulent kinetic energy (TKE), both normalized by $\mathcal{V}_{mode}^2$. The normalization yields a dimensionless measure of fluctuation strength relative to the *a priori* predictor based on the Stokes settling velocity. In the absence of fluctuations, the domain approaches the Stokes regime. Shown in Figure 4.3 (a), is the data collected from the present study overlaid with data reported by Capecelatro et al. [79]. The fluid-phase TKE, k_f , increased almost linearly with increasing domain size for the polydisperse assemblies of particles. The test cases from [79] follow a similar trend line but have a less steep increase. This can be attributed to the larger degree of clustering and settling speeds observed in the polydisperse configurations relative to the monodisperse cases. The presence of clusters results in larger velocity fluctuations in the fluid-phase. In contrast,

the total fluctuating granular energy remains nearly constant across the domains studied in this work. This is consistent with the degree of clustering, $\mathcal{D}$, that was also observed.

Lastly, the relative contributions of particle-phase TKE and granular temperature to the total granular energy are examined, together with the magnitude of the fluid-phase TKE relative to the total granular energy. Figure 4.3 (b) shows data from the present study as well as data from [79]. In each domain studied, the fluid-phase TKE, k_f , exceeds that of the particle-phase TKE, which is consistent with the trend observed in the monodisperse study. Here, the PA granular temperature makes up about 75% of the total granular energy, while the remaining 25% is attributed to the particle-phase TKE (greater contribution from unresolved TKE). This trend is the opposite of what was observed in previous monodisperse studies and is likely attributable to the filtering operation used in the polydisperse work. Filtering strategies will be discussed further in Chapter 5.

Following [79], a constant filter width of $7d_{p,10}$ was applied to the configurations in both the monodisperse and polydisperse configurations. Because the particle population is polydisperse, no single filter width can adequately resolve the full range of particle scales. Consequently, the selected filter may not fully capture the particle-phase TKE associated with the smallest particles. Finally, the contributions of the particle-phase TKE and granular temperature to the total granular energy remain fairly constant for the configurations studied. These results may therefore depend on the chosen filtering approach.

4.3 CONCLUSIONS

In this study, how domain size influences fluid–particle steady-state statistics in increasingly large simulation domains composed of *polydisperse* particles was investigated. Three domain configurations were considered, and the resulting statistics were compared against established results from monodisperse simulations [79]. In agreement with the study conducted in Chapter 3, the presence of a polydisperse particle size distribution leads to stronger clustering behavior, which in turn promotes higher settling velocities and elevated levels of fluid-phase TKE.

The results further indicate that domain scaling can be effectively performed using a characteristic particle diameter defined by the mode of the size distribution. Based on this scaling, domains corresponding to configuration 3 and larger appear sufficient to capture the relevant flow physics. These results may depend on filter size, as discussed in the following chapter.

These observations have direct relevance for the development of sub-grid scale (SGS) models in coarse-grained Euler–Euler simulations. Because clustering, mean settling velocity, and phase turbulence depend on domain size, SGS closures should be developed using domains that capture statistically steady two-phase dynamics or incorporate appropriate scaling laws, such as those based on the modal particle diameter.

CHAPTER 5

THE EFFECT OF FILTER SIZE ON FLUID-PARTICLE STATISTICS IN POLYDISPERSE MULTIPHASE GAS-SOLID FLOWS

5.1 INTRODUCTION

Coarse-grained multiphase simulations are inherently influenced by the selected filtering or averaging scale. Despite this dependence, many existing closure formulations do not explicitly account for the effects of grid or filter size, motivating the development of improved closures that remain applicable across varying spatial and temporal scales. Filtering procedures used to map Lagrangian particle data onto an Eulerian framework therefore play a critical role in closure development for coarse-grained solvers by introducing several unresolved quantities that require additional modeling, including interphase drag, mean slip velocity, and unresolved particle-phase energy fluctuations. This work focuses primarily on modeling these unresolved energy fluctuations.

Previous numerical studies have demonstrated that multiphase turbulence statistics are strongly influenced by the selected filter size [202–206]. Appropriate filtering procedures are therefore necessary to ensure that steady-state quantities, including settling velocity, volume-fraction fluctuation statistics, and particle-phase energy fluctuations, remain physically representative and are not artificially affected by the filtering operation.

When Lagrangian particle information is projected onto an Eulerian mesh and spatially smoothed, a portion of the particle-scale fluctuating motion becomes unresolved.

This unresolved fluctuating energy is commonly referred to as granular temperature [212] (refer to Section 2.0.1.4). Granular temperature contributes significantly to the total granular energy associated with particle velocity fluctuations. This work focuses on developing a filter-dependent model for granular temperature in polydisperse flows. The resulting formulation is intended for extension to TFM solvers, where the filter size may be related directly to the coarse-grid resolution.

5.2 METHODOLOGY

To examine these effects of filtering strategy on polydisperse flows, two lognormally distributed particle assemblies at two different volume fractions are considered, and filters of progressively increasing size are systematically applied to statistically stationary flow data for each configuration, as described in the following sections.

Throughout this study, comparisons are made with two closely related investigations. In particular, Capecelatro [79] examined multiphase turbulence statistics using both fixed and adaptive filtering approaches in *monodisperse* suspensions. More recently, Rosenberg [213] developed a filter-dependent formulation for granular temperature using an extensive set of highly resolved gas-solid simulations spanning conditions from very dilute systems to near close-packing. These studies provide a foundation for this analysis.

This study extends these previous efforts to *polydisperse* suspensions containing particles that are, on average, significantly larger than those considered in Capecelatro

[214] and Rosenberg [213], which focused primarily on particles near $90 \mu\text{m}$ in diameter. Here, particle diameters range from $27 \mu\text{m}$ to 3 mm . This expanded parameter space provides additional insight into how fixed and adaptive filtering procedures influence multiphase turbulence statistics in highly polydisperse systems.

5.2.1 SYSTEM DESCRIPTION

Configuration parameters are equivalent to the polydisperse cases studied in Chapter 3 and are denoted as A and B throughout this study. Recalling that distribution A is shifted toward larger particle diameters, resulting in fewer particles for a given mass loading, and, in contrast, Distribution B is shifted toward smaller particle diameters, yielding a larger particle count.

5.2.2 INTERPHASE COUPLING STRATEGY

The two-step filtering technique discussed in Chapter 2 is employed on each configuration under study. Filter size, δ_f , affects turbulence statistics in multiphase flows, specifically in the context of averaging particle velocities. To highlight this, recall that the total particle-phase fluctuating energy κ_p , defined in Eq. (2.19), is a sum of the correlated and uncorrelated particle velocity fluctuations and therefore is affected by filter size selection.

If the filter size is much larger than the mean particle diameter, i.e., $\delta_f \gg d_p$, the instantaneous particle velocity $\mathbf{u}_p$ approaches the filtered mean velocity $\langle \mathbf{u}_p \rangle_f$. As a result, fluctuations about the filtered field are strongly suppressed, leading to $k_p \approx 0$. In this limit, the total granular energy κ_p is dominated by the uncorrelated particle fluctuations

represented by Θ , which correspond to sub-filter contributions that are not resolved on the Eulerian mesh.

If the filter size is comparable to the particle diameter, i.e., $\delta_f \approx d_p$, the filter preserves a significant portion of the particle velocity fluctuations. In this case, both the correlated and uncorrelated particle velocities contribute to the total granular energy κ_p .

If the filter size is significantly small, i.e., $\delta_f \ll d_p$, only the initial extrapolation step of the filtering process is effectively performed, and the resulting fields may become noisy or poorly defined due to insufficient particle information within the filter volume. Previous work [79] demonstrated that for monodisperse particles, a filter size of $1.75 d_{p,10}$ is the smallest filter size that ensures accurate steady-state flow statistics; however, it is unclear whether or how this extends to assemblies of particles that are polydisperse.

To obtain meaningful data from steady-state simulation results, the calculated statistics should be independent of the averaging volume employed, meaning that the computed values (e.g., particle concentration, velocity, volume fraction) should not be significantly influenced by the size of the region used for averaging. If the volume is too small or the sample size is too low, there will be high fluctuations and unreliable statistics. If the volume is too large, local details may be lost, leading to overly smoothed results. The goal is to find a balance where statistical results do not change significantly when the averaging volume is varied. Instead of using a fixed averaging volume across the entire domain, an adaptive volume method can be used. In this method, the size of the averaging region is adjusted based on the local particle concentration (i.e., in dilute regions of the

flow, the volume is increased to ensure enough particles are sampled for reliable statistics, and in dense clusters, the volume remains compact to capture fine-scale details). Under these conditions, the number of particles sampled, $\mathcal{N}_p$, determines how large the averaging volume is.

$$\delta_f(\alpha_p) = \left(\frac{\mathcal{N}_p d_p^3}{\alpha_p} \right)^{1/3} \quad (5.1)$$

Similar studies have been conducted on monodisperse assemblies of particles [79]. In the case of uniform-sized particles, $\mathcal{N}_p$ will be a constant, and the filter width, δ_f , will be the same for each particle.

5.3 RESULTS

Two filtering approaches were investigated to evaluate their influence on granular temperature in polydisperse gas-solid flows: fixed and adaptive filtering. Fixed filters provide a direct analog to TFM methodologies, where increasing filter size corresponds to progressively coarser computational grids. Adaptive filtering, by comparison, has been shown to improve the balance between statistical convergence and excessive smoothing by allowing the filter size to vary throughout the domain in order to maintain a sufficient number of particles within each averaging volume [81]. This adaptive strategy is also conceptually consistent with PIC-type approaches, in which each computational parcel contains a prescribed distribution of particles. In this sense, the effective filtering behavior

evolves according to parcel dynamics rather than being determined solely by the spatial mesh resolution.

Previous studies have shown that increasing filter size shifts a larger fraction of the total granular energy into the unresolved component, $\langle \Theta_p \rangle$, thereby increasing the dependence on closure modeling [213]. However, these effects have not yet been quantified directly for highly polydisperse particle assemblies.

Steady-state slices of each configuration under study are shown in Figure 5.1. Fluid-phase velocity (grayscale) is normalized with the polydisperse Stokes velocity for that distribution, $\mathcal{V}_{0,10}$, and particles are colored by diameter (from blue (small) to yellow (large) for Distribution *A* and from pink (small) to red (large) for Distribution *B*).

5.3.1 FIXED FILTERING STRATEGY

In this section, the effect of fixed filtering on granular temperature is considered. In particular, 19 filters of increasing size were applied to each of the highly resolved E-L datasets. These filter sizes are bounded by $\delta_f = 0.1d_{p,10}$ and $\delta_f = 26d_{p,10}$.

Two important quantities of interest are considered: first, the degree of clustering that is captured as a function of filter size, followed by an analysis of the granular energy and a filter-dependent model for granular temperature.

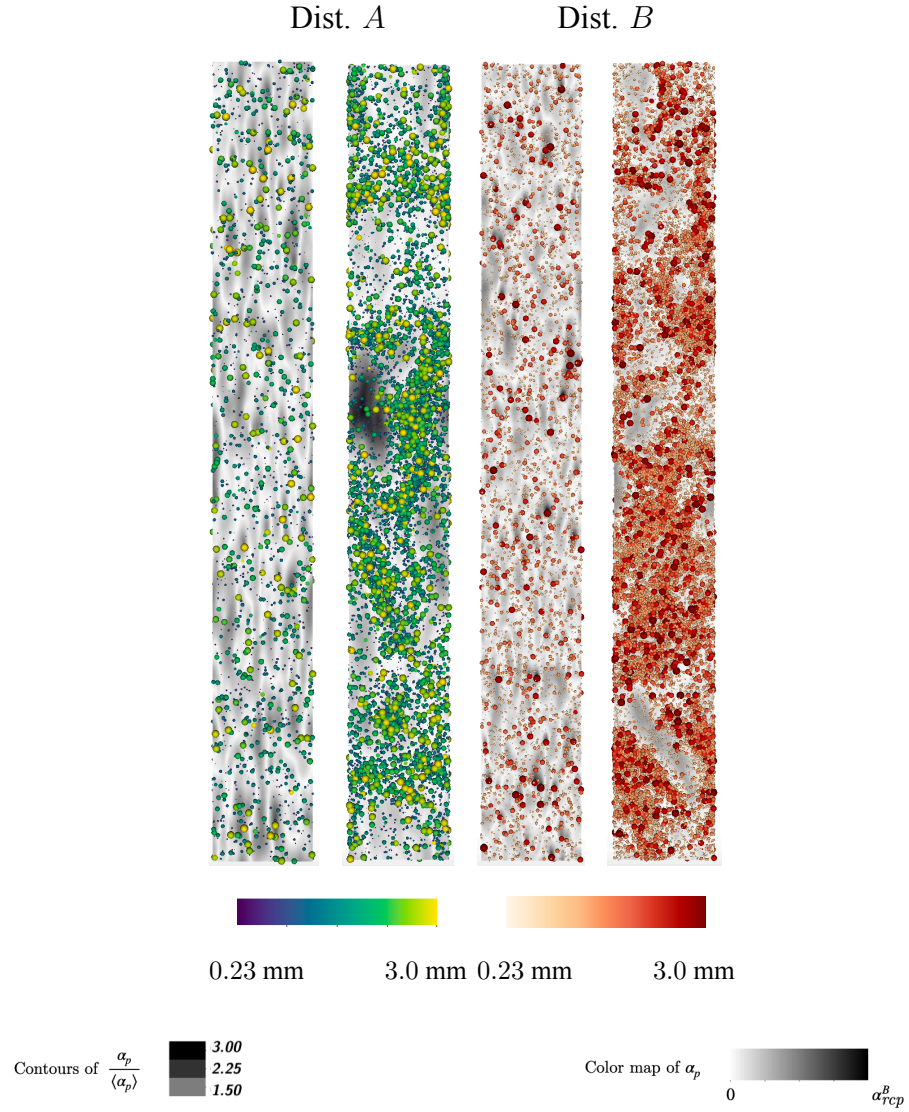


Figure 5.1: Representative snapshots from the statistically stationary period of each configuration. Each slice is an x - y plane at $z = 0$. Fluid-phase velocity (grayscale) is normalized by the polydisperse Stokes velocity for that distribution, $\mathcal{V}_{0,10}$, and particles are colored by diameter (from blue (small) to yellow (large) for Distribution A and from pink (small) to red (large) for Distribution B).

5.3.1.1 PARTICLE CLUSTERING BEHAVIOR For gas-solid flows with sufficiently large mass loading, quantifying the extent of particle clustering is essential for characterizing overall flow behavior. Accordingly, this section evaluates the degree of

clustering for each of the four configurations considered in the present study as a function of filter size.

Figure 5.2 illustrates the effect of increasing filter size on the distribution of the local volume fraction, α_p , for the four steady-state configurations under consideration. The top two rows represent Dist. *A* ($\langle\alpha_p\rangle = 0.01$, row one, and $\langle\alpha_p\rangle = 0.10$, row two) and the bottom two similarly represent Dist. *B*. Each column represents a progressively larger filter width, ranging from $\delta_f = 0.1d_{p,10}$ to $22d_{p,10}$. The grayscale fields depict $\langle\alpha_p\rangle$ in an x-y plane at $z = 0$, with darker shades indicating regions of higher local concentration.

At the smallest filter widths, the configurations contain numerous localized peaks and larger regions void of clusters. This result, though intuitive, is due to *less* smoothing (smaller area being smoothed) being applied to the extrapolated Lagrangian quantities. As δ_f increases, the small-scale fluctuations are increasingly smoothed, and the contrast between dense and dilute regions diminishes, resulting in a more homogeneous field. This trend is consistent with a larger filter size area.

Comparison across configurations highlights the influence of particle size distribution and quantity. Polydisperse cases with smaller particles (Dist. *B*) exhibit denser regions of clusters, particularly when $\langle\alpha_p\rangle = 0.01$, implying that Dist. *B* experiences enhanced clustering, which is consistent with the results reported in Foster [78]. In each configuration, the low volume fraction cases exhibit a sharper difference in clustering concentration when compared to the higher volume fraction cases that appear to be smoother.

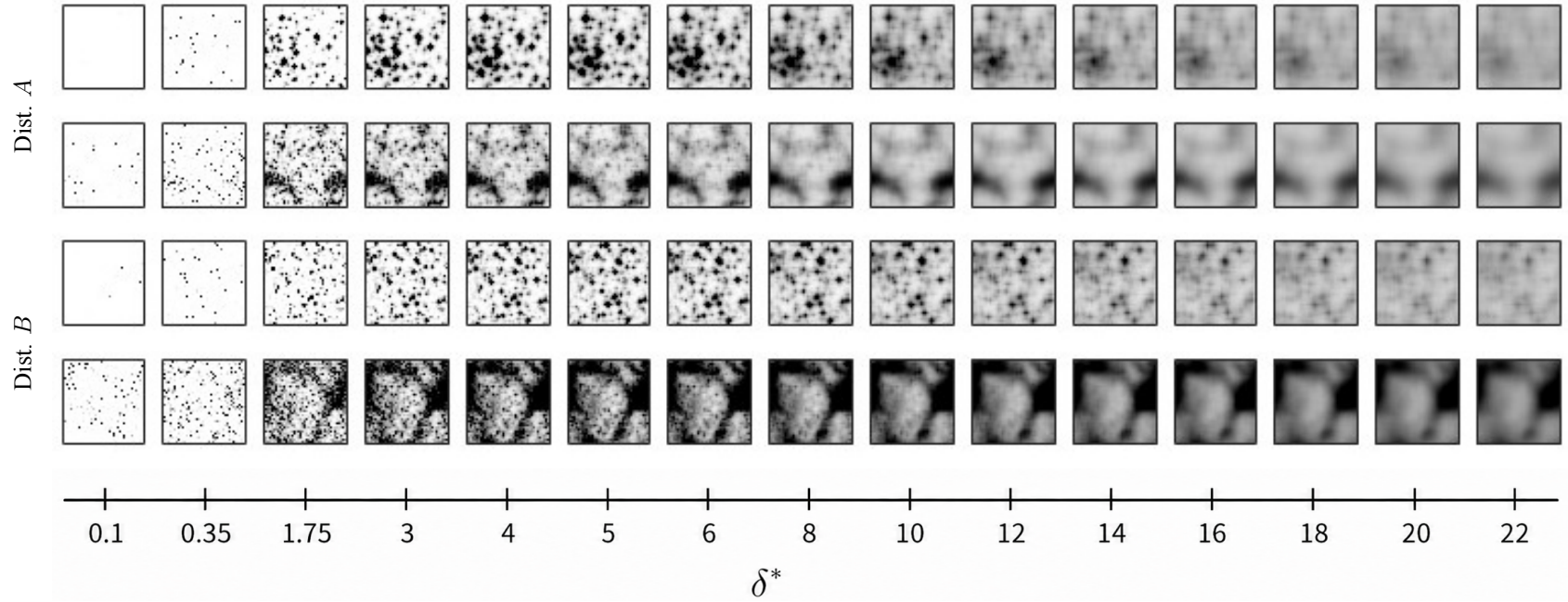


Figure 5.2: Representative snapshots from the statistically stationary period of each configuration. From top to bottom Dist A $\langle \alpha_p \rangle = 0.01$, Dist. A $\langle \alpha_p \rangle = 0.1$, Dist. B $\langle \alpha_p \rangle = 0.01$, Dist. B $\langle \alpha_p \rangle = 0.1$. Each slice is an x - y plane at $z = 0$. local volume fraction $\langle \alpha_p \rangle$ (grayscale) for each configuration, ranging from 0 (white) to the global $3\langle \alpha_p \rangle$, is plotted against the fixed filter sizes under study (left to right) $\delta_f = (0.1, 0.35, 1.75, 3, 4, 5, 6, 8, 10, 12, 14, 16, 18, 20, 22)$ $d_{p,10}$.

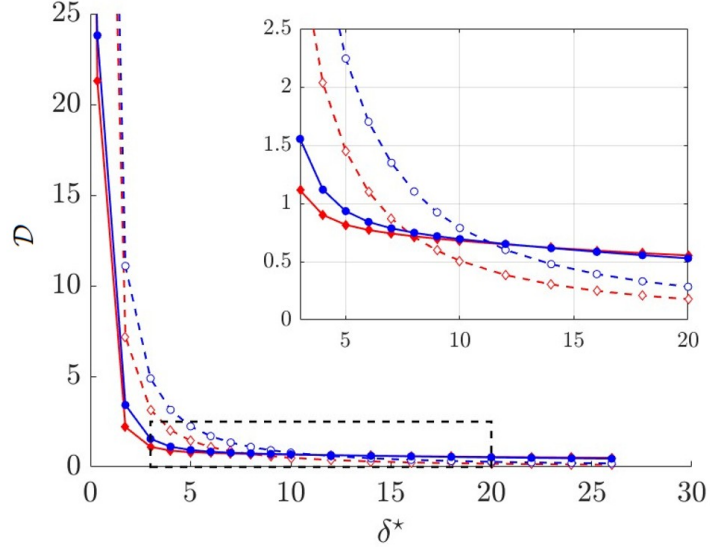


Figure 5.3: Summary of degree of clustering, $\mathcal{D}$, for all configurations under study. Red denotes Dist. *A* and blue denotes Dist. *B*. Open and filled markers, as well as dense and dashed lines, represent the dilute and dense cases, respectively.

The mean variance in volume fraction to quantify the degree of clustering as defined in Chapter 3 is also leveraged. For all cases, $\mathcal{D}$ decreases monotonically with increasing δ_f , following the trend shown in Figure 5.2. Figure 5.3 displays the degree of clustering with respect to normalized filter size, wherein $\delta^* = \delta_f/d_{p,10}$. Intuitively, when $\mathcal{D}$ is larger, the fluid fields will contain larger structures and larger areas void of particles. As δ_f increases, these localized peaks are averaged out, and the degree of clustering approaches zero, corresponding to a nearly random particle distribution. In this limit, a model for the degree of clustering is then required due to over-smoothing. The degree of clustering is overall higher in the dilute cases, specifically that of Dist. *B*, which is consistent with previous work from Foster [78].

5.3.1.2 PARTICLE-PHASE FLUCTUATING ENERGY BEHAVIOR This section examines how filtering influences the partitioning of total granular energy between resolved and unresolved particle velocity fluctuations. Particular attention is given to the fraction of granular energy represented by the resolved particle-phase turbulent kinetic energy, k_p , relative to the unresolved contribution contained within the granular temperature, $\langle\Theta\rangle_p$, which must ultimately be represented through closure modeling.

Figure 5.4 presents the contributions of k_p and $3\langle\Theta\rangle_p/2$ to the total granular energy as a function of normalized filter size. As the filter width, δ_f , increases, the resolved component k_p decreases steadily, indicating that progressively larger filters smooth out particle velocity fluctuations that are otherwise retained at smaller filter sizes. Consequently, an increasing portion of the total granular energy becomes unresolved and is transferred into the granular temperature contribution.

For each configuration, a characteristic filter size, denoted δ_{50}^* , is identified where the unresolved granular energy contribution exceeds the resolved component (measured at the intersection of the lines for particle TKE and granular temperature). However, this transition point remains relatively similar between Dist. *A* and Dist. *B*; it exhibits a strong dependence on particle volume fraction, consistent with the observations of Rosenberg [213]. Specifically, δ_{50}^* was found to be 3.95 and 4.97 for the dilute Dist. *A* and Dist. *B* cases, respectively, and 16.01 and 18.68 for the corresponding dense cases.

These findings have important implications for grid-resolution requirements in coarse-grained approaches such as TFM. In particular, the results suggest that dilute flows require finer computational grids than dense flows in order to retain a comparable fraction of resolved granular energy and maintain a similar dependence on closure modeling for the unresolved granular temperature. Motivated by these observations, a filter-dependent model for granular temperature was proposed.

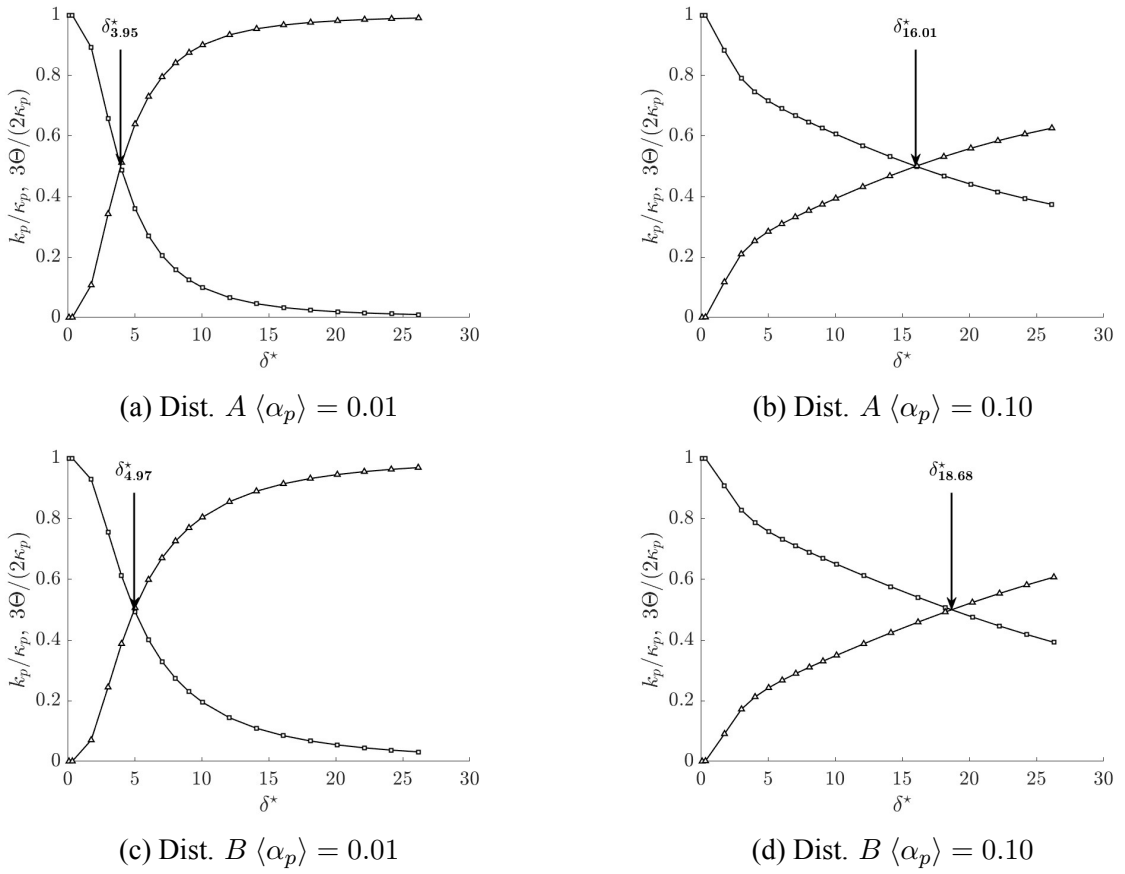


Figure 5.4: Relative contributions to the total granular energy normalized by total granular energy as a function of normalized filter size. The relative resolved contribution, k_p/κ_p , is denoted by squares, and $3\langle\Theta\rangle_p/(2\kappa_p)$ is denoted by triangles. The intersection of these contributions is denoted as δ^*_{50} .

5.3.2 A FILTER-DEPENDENT CLOSURE FOR GRANULAR TEMPERATURE

As leveraged in the recent work of Rosenberg [213], a PR-DNS-based model for granular temperature was proposed by Tang [215] as a function of Reynolds number.

$$\text{Re}_\Theta = \frac{\rho_f d_{p,10} \sqrt{\langle \Theta \rangle_p}}{\mu_f}, \quad (5.2)$$

with the model for Re_Θ given as,

$$\text{Re}_\Theta \left(\text{Re}_p, \frac{\rho_p}{\rho_f} \right) = 2.108 \text{Re}_p^{0.85} \left(\frac{\rho_p}{\rho_f} \right)^{-0.5}, \quad (5.3)$$

and with Re_p , the particle Reynolds number, defined as

$$\text{Re}_p = \frac{\rho_f d_{p,10} (1 - \langle \alpha_p \rangle) |\langle u_p \rangle - \langle u_f \rangle|}{\mu_f}. \quad (5.4)$$

A preliminary investigation by Raval and Fullmer [216] demonstrated that the functional relationship originally proposed by Tang et al. [215] remains valid even when applied to the significantly larger CIT dataset. This was further bolstered in the study conducted by Rosenberg [213]. However, the numerical values of the leading coefficient and exponent required modification. Their analysis also indicated that these adjustments depend on whether a spatial filter is applied. In this study, a broad range of filter sizes,

introduced earlier, is examined, and the objective is to represent these coefficients as continuous functions of the filter size. Accordingly, the relationship is modeled as

$$\text{Re}_\Theta(\delta^*) = A_\Theta(\delta^*) \text{Re}_p^{B_\Theta(\delta^*)} \left(\frac{\rho_p}{\rho_f} \right)^{-0.5}. \quad (5.5)$$

Where A_Θ and B_Θ are functions dependent of normalized filter size, δ^* .

In this study, Re_Θ and Re_p were computed based on collected steady-state data for each configuration. Due to the triply periodic nature of the simulations, the mean settling velocities remained relatively similar across the four configurations. The mean settling velocities for Dist. *A* were -0.20 and -0.16 m/s for the dilute and dense cases, respectively, while those for Dist. *B* were -0.19 and -0.10 m/s. As a result, each configuration was characterized by a nearly constant particle Reynolds number, with $\text{Re}_p = 6.2, 4.27, 2.15$, and 1.59 for the dilute and dense configurations of Dist. *A* and Dist. *B*, respectively. This yielded four distinct closures for A_Θ and B_Θ , one for each distribution studied, as described in Eqs. (5.6) and (5.7), respectively. Table 5.1 summarizes the constant coefficients leveraged in the proposed equations for A_Θ and B_Θ .

$$A_\Theta(\delta^*) = (1 - e^{-k_0\delta^*}) (a_1\delta^* + a_0) \quad (5.6)$$

$$B_\Theta(\delta^*) = b_1e^{-k_1\delta^*} + b_2e^{-k_2\delta^*}. \quad (5.7)$$

Shown in Figure 5.5 is the resulting model wherein the loosely dashed line represents the dilute configurations and a solid line denotes the dense configurations.

Table 5.1: Summary of fitted model coefficients for each particle distribution and volume fraction configuration studied.

$\langle \alpha_p \rangle$	Dist.	a_0	a_1	b_1	b_2	k_0	k_1	k_2
0.01	A	-0.32	1.77	1.48	-0.48	1.01	0.063	0
	B	12.18	0.04	0.49	-3.03	0.28	0.00	1.10
0.10	A	40.72	-0.54	1.33	-2.02	0.56	0	0
	B	20.97	-0.23	2.22	-4.27	0.61	0	0.02

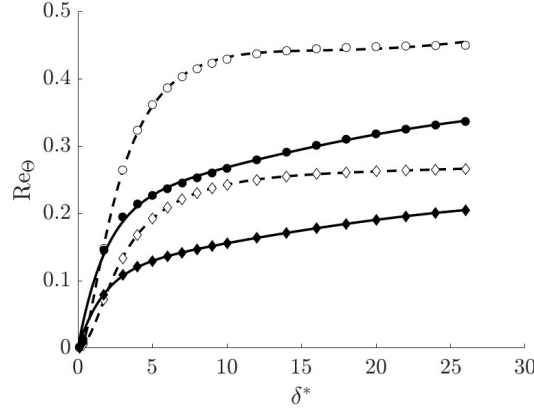
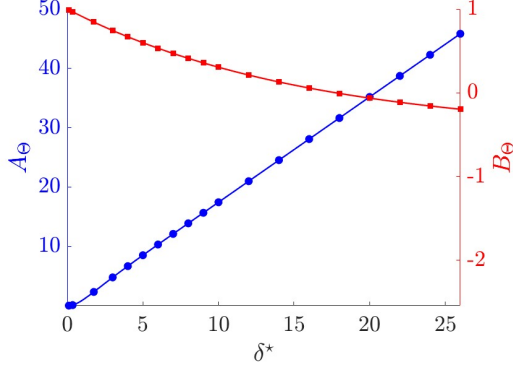


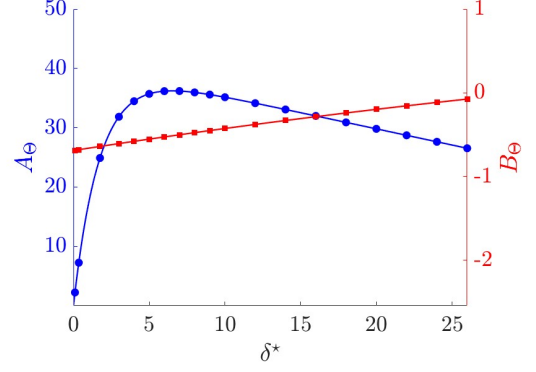
Figure 5.5: The dashed line represents the dilute cases from model (5.5) and the solid line denotes the dense distributions. Circles represent Dist. A and diamonds represent Dist. B. Solid markers denote $\langle \alpha \rangle = 0.10$ and open markers denote $\langle \alpha \rangle = 0.01$. Note that the average root-mean-squared error is 0.003.

Circles represent Dist. A and diamonds represent Dist. B. Solid markers denote $\langle \alpha \rangle = 0.10$ and open markers denote $\langle \alpha \rangle = 0.01$. The proposed model accurately predicts the data computed in this study, wherein the average root mean squared error is 0.003.

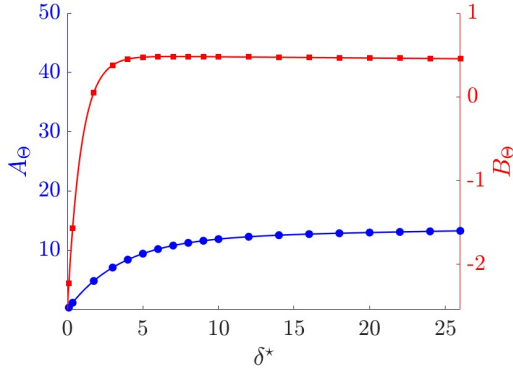
Figure 5.6 illustrates the dependence of the fitted model coefficients A_Θ and B_Θ on the normalized filter size, δ^* , for each configuration studied. The dense configurations, shown in Figure 5.6 (b,d), exhibit comparatively similar coefficient trends despite differences in particle distribution. In both cases, A_Θ initially increases rapidly before gradually decreasing or plateauing, while B_Θ varies more smoothly with filter size. In



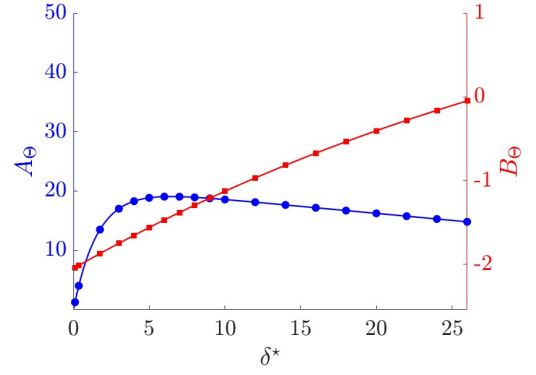
(a) Dist. A $\langle \alpha_p \rangle = 0.01$



(b) Dist. A $\langle \alpha_p \rangle = 0.10$



(c) Dist. B $\langle \alpha_p \rangle = 0.01$



(d) Dist. B $\langle \alpha_p \rangle = 0.10$

Figure 5.6: Model coefficients with respect to normalized filter size for each configuration studied. Here, the model coefficient A_Θ is shown in blue and B_Θ is shown in red.

contrast, the dilute configurations, shown in Figure 5.6 (a,c), display significantly different trends between the two particle distributions. For Dist. A at $\langle \alpha_p \rangle = 0.01$, A_Θ increases nearly linearly with δ^* while B_Θ decreases gradually. Conversely, Dist. B at $\langle \alpha_p \rangle = 0.01$ shows a rapid increase in B_Θ that gradually levels off, along with a relatively small increase in A_Θ . These differences indicate that the dilute cases are more sensitive to variations in particle Reynolds number and particle size distribution.

The functional form of the proposed models in this work, as well as that of Rosenberg [213], are identical. However, an important distinction exists between the two

studies. In the monodisperse study, the particle diameter was held constant while the particle Reynolds number, Re_p , varied across the cases considered. As a result, the fitted model exhibited a strong dependence on Re_p . In the present work, the opposite approach is taken, where Re_p remains approximately constant within each configuration while the particle size distribution varies. Consequently, the fitted coefficient functions A_Θ and B_Θ exhibit substantially different behavior compared to the monodisperse study. In particular, the trends of the coefficients appear effectively reversed, with A_Θ displaying a stronger nonlinear or exponential dependence on δ^* in most cases, while B_Θ varies more linearly. This contrasts with the findings of Rosenberg [213], where A_Θ exhibited a more linear dependence and B_Θ showed stronger nonlinear behavior. Nonetheless, the model for Re_Θ in the monodisperse study and this work show similar trends in which Re_Θ increases with normalized filter size and eventually reaches an asymptotic limit.

The functional form of Eq. (5.5) was selected to preserve the Reynolds-number dependence proposed by Tang et al. [215], allowing direct comparison between the present polydisperse closures and the previous monodisperse study [213]. Rather than modifying the underlying model, the filter-size dependence was incorporated through the coefficients A_Θ and B_Θ . The functional forms of Eqs. (5.6) and (5.7) were chosen because they provided accurate representations of the observed variation with normalized filter size while remaining sufficiently simple for implementation. Unlike the closure models proposed in the previous sections, these expressions were not constructed to satisfy any prescribed physical limits or asymptotic behavior. Instead, the coefficients $a_0, a_1, b_1, b_2,$

k_0 , k_1 , and k_2 were determined solely by nonlinear curve fitting to the simulation data.

Consequently, the proposed relationships should be interpreted as empirical correlations that are valid over the range of filter sizes investigated in this study.

5.3.3 ADAPTIVE FILTERING STRATEGY

In this section, the results of the adaptive filtering approach described in Section 5.2.2 are presented. The purpose of the adaptive filter is to maintain a consistent number of particles within the filtering volume as the local particle concentration changes.

Therefore, the filter size is not prescribed independently; instead, it is selected based on the expected number of particles, $\mathcal{N}_p$, contained within the filter.

From Eq. (5.1), the expected number of particles within a cubic filtering volume scales as the ratio of the filter volume to the particle volume, weighted by the local particle volume fraction. Assuming a characteristic particle diameter, d_p , this scaling may be written as

$$\mathcal{N}_p \sim \langle \alpha_p \rangle \left(\frac{\delta_f}{d_p} \right)^3. \quad (5.8)$$

Rearranging Eq. (5.1) as Eq. (5.9) allows a closer comparison to the fixed filter size, by allowing the expected number of particles to be estimated in advance from the prescribed filter width and the mean particle volume fraction. This estimate provides a useful reference for selecting the target number of particles used in the adaptive filtering procedure.

$$\delta_f(\langle\alpha_p\rangle) = \left(\frac{\mathcal{N}_p}{\langle\alpha_p\rangle}\right)^{1/3} d_p. \quad (5.9)$$

In the following results, target values of $\mathcal{N}_p$ are selected for each configuration to evaluate the sensitivity of the filtered quantities to the number of particles included in the adaptive filtering volume.

5.3.3.1 PARTICLE-PHASE FLUCTUATING ENERGY BEHAVIOR In this section, the total particle phase energy is evaluated and compared to that in the fixed filter evaluation discussed in Section 5.3.1.

Figure 5.7 details the results of both the fixed (shown by a dense line with closed markers) and adaptive (shown by a dashed line with open markers) contributions of the total fluctuating energy of the particle-phase and granular temperature to the overall granular energy at each normalized filter size. Note that for the adaptive filter strategy, the nominal $\langle\alpha_p\rangle$ is used in Eq. (5.1) to mathematically formulate a relationship between the fixed and adaptive configurations in the form of $\delta^* = \delta_f/d_{p,10}$.

It can be seen that the adaptive and fixed filters have very similar curves for the contributions to the total granular energy. The dilute cases under study require a smaller particle sample size, $\mathcal{N}_p$, when compared to the dense cases. This trend is consistent with the values reported for the fixed filter.

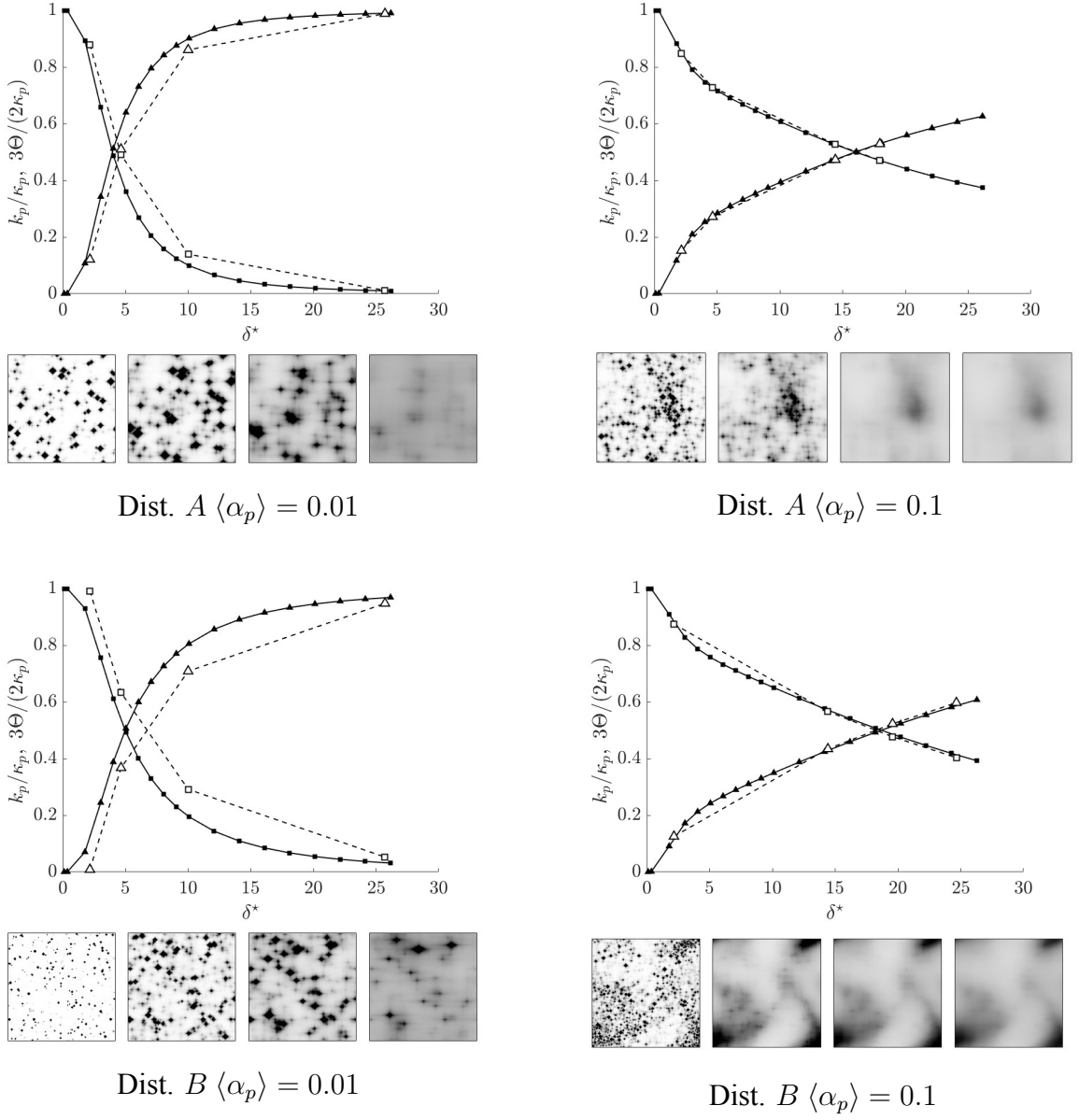


Figure 5.7: Separate contributions to the total granular energy normalized by κ_p wherein k_p is denoted by squares and Θ is denoted with triangles as a function of normalized filter size δ^* . The dashed line represents the adaptive filter, and the solid line represents the fixed filter. Representative snapshots from the statistically stationary period of each configuration of local volume fraction $\langle \alpha_p \rangle$ (grayscale) for each configuration, ranging from 0 (white) to $3\langle \alpha_p \rangle$, are shown against the adaptive filter sizes under study (left to right), described by Dist. A $\langle \alpha_p \rangle = 0.01$ with $\mathcal{N}_p = 0.01, 1, 10, 170$, Dist. A $\langle \alpha_p \rangle = 0.1$ with $\mathcal{N}_p = 1, 1, 10, 300, 508$, Dist. B $\langle \alpha_p \rangle = 0.01$ with $\mathcal{N}_p = 0.01, 1, 10, 170$, and Dist. B $\langle \alpha_p \rangle = 0.1$ with $\mathcal{N}_p = 1, 300, 750, 1500$. Each slice is an x - y plane at $z = 0$.

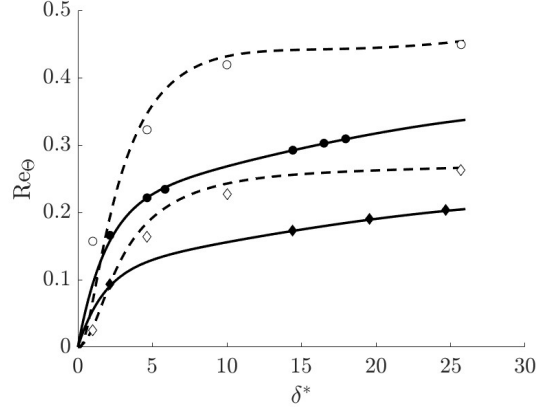


Figure 5.8: The dashed line represents the dilute case from model (5.5) and the solid line denotes the dense distributions based on the fixed filter. Circles represent Dist. A and diamonds represent Dist. B . Solid markers denote $\langle \alpha \rangle = 0.10$ and open markers denote $\langle \alpha \rangle = 0.01$ for the adaptive filter. Note that the overall root-mean-squared error is 0.03.

To further demonstrate this similarity, the granular temperature model developed using fixed-filter steady-state statistics, given by Eq. (5.5), is compared with the steady-state statistics obtained using the adaptive filter.

Shown in Figure 5.8 is the adaptive filter data versus the fixed filter model curves formulated in Section 5.3.2. The model captures the general behavior of the steady-state data, although the agreement is less favorable than that observed for the fixed filter. The overall root-mean-squared error is 0.03.

5.4 CONCLUSIONS

The results presented thus far demonstrate that filter sizes can strongly influence two-point steady-state statistics. When the filter is much larger than the particle diameter ($\delta_f \gg d_p$), the particle velocities are heavily smoothed, and the fluctuations are essentially removed, so $k_p \approx 0$ and the granular energy is dominated by the unresolved, particle-scale

motion captured by Θ . When the filter is on the order of the particle diameter ($\delta_f \approx d_p$), a good portion of the particle fluctuations are preserved, so both the correlated motion (k_p) and the uncorrelated motion (Θ) contribute to κ_p . If the filter is much smaller than the particle diameter ($\delta_f \ll d_p$), the filtering does not do much beyond the initial extrapolation step, and the resulting fields tend to be noisy or poorly defined because there are not enough particles in the filter volume.

Both fixed and adaptive filtering strategies were verified, and it was determined that the adaptive filter can provide accurate two-point steady-state statistics, provided that the particle sample size is not too large or too small. The use of the fixed filter is also feasible for such results. The results presented in this chapter indicate that the selection of an appropriate filter size represents a tradeoff between computational cost and physical fidelity. Smaller filters resolve a greater portion of the particle-phase fluctuations, thereby reducing the contribution of unresolved sub-filter-scale motions, whereas larger filters decrease the computational expense at the cost of requiring more comprehensive closure models to represent the unresolved dynamics. As a result, no single filter size is optimal for all applications. Rather, the appropriate filter width depends on the desired balance between the resolved and unresolved components of the flow and the level of accuracy required for the intended application.

An analysis of a PR-DNS model for granular temperature, introduced by [215], was conducted. It was found that such modeling did not accurately predict large-scale behavior such as clustering. An alternate formulation of the mathematical description in

Tang [213, 215] was proposed, which was developed wherein the leading coefficients were modified for filter-dependent closures.

Overall, this work represents an initial step toward developing improved closures for coarse-grained solvers, particularly particle-in-cell (PIC) and Euler–Euler (EE) frameworks. In EE models, where both phases are treated as continua, closures are required to represent unresolved particle-scale physics, including collisions, velocity fluctuations, and clustering. The present work addresses this need by introducing a filter-dependent closure relating unresolved particle velocity fluctuations to Reynolds number, which can be predicted *a priori*. In PIC methods, where particles are tracked as parcels and coupled to an Eulerian grid, closures are similarly needed to account for unresolved particle interactions and velocity fluctuations arising from parcel averaging [36, 217, 218]. Developing filter-dependent drag closures is also important, as drag governs momentum exchange between the fluid and particle phases.

CHAPTER 6

SUMMARY AND FUTURE OUTLOOK

6.1 SUMMARY

This work analyzed the settling and clustering behavior of polydisperse gas-solid flows. It resulted in six key outcomes: (1) A new measure called *surface loading* to predict the degree of clustering and settling behavior, (2) a model closure for fluid velocity, (3) a model for mean particle settling velocity, (4) a new drag model that accurately predicts settling velocity across particle sizes that includes effects of clustering, (5) established a logarithmic relationship for domain size scaling (characteristic cluster length) and particle settling, and (6) a proposed model for predicting granular temperature as a function of particle Reynolds number and filter size.

Chapter 3 analyzed two polydisperse configurations as well as two monodisperse analogs at two different volume fractions, resulting in 8 configurations. The implications of particle size polydispersity on clustering behavior and steady-state settling velocity were analyzed. The results were compared with monodisperse studies as well as common models used in volcanology. Overall, it was found that polydispersity in a system results in a greater degree of clustering because smaller particles can fill voids that would otherwise remain in a monodisperse assembly. The deviation in volume fraction is commonly used to explain the degree of clustering in monodisperse systems. It was shown to be an inaccurate predictor for a polydisperse ensemble. As a result, a new

measure called *surface loading*, which leverages the mean surface diameter of particles, was proposed to predict the degree of clustering. It was also found that polydispersity increases particle settling velocity and that using *a priori* predictors such as Stokes settling law did not accurately predict the observed settling speeds. *Surface loading* was once again leveraged to create a new *a priori* for particle settling velocity. Lastly, a comparison was drawn between existing *a priori* settling velocity predictors used in volcanology. Though able to predict settling velocity better than Stokes, the methodology did not take into account particle clustering. A new drag model that accurately predicts settling velocity across particle sizes, which includes the effects of clustering, was presented.

Chapter 4 analyzed 3 increasingly larger simulation domains and the effects of domain scaling on various quantities of interest, such as particle settling velocity, degree of clustering, and velocity fluctuations in both the particle and fluid phases. The results were compared to equivalent monodisperse studies. The domains studied were in agreement with monodisperse simulations. It was found, though, that existing scaling predictors did not accurately predict particle settling velocity in polydisperse systems. This is due to existing scaling laws leveraging particle diameter, which in this case varies. Scaling was investigated using statistical diameters as well as the minimum and maximum particle diameters. It was found that using the modal diameter produced the best domain scaling relationship. As a result, a logarithmic predictive relationship for domain size scaling (characteristic cluster length) and particle settling was established.

Chapter 5 analyzed the effects of filtering strategy, both fixed and dynamic, on steady-state statistics with a focus on particle-phase TKE and granular temperature. A total of 19 fixed and 8 adaptive filter sizes were evaluated for two polydisperse particle assemblies. The results were compared to monodisperse studies. It was found that polydispersity alters the smallest plausible filter size feasible for reliable results established in the monodisperse studies. It was also found that granular temperature was sensitive to filter size. As a result, a model was developed to calculate the granular temperature *a priori* based on the particle Reynolds number and filter size. This model was validated using both fixed- and adaptive-filtering steady-state statistics.

6.2 FUTURE WORK

6.2.1 INTEGRATION INTO LARGE-SCALE SOLVERS

The closure relationships developed throughout this dissertation demonstrate that key unresolved multiphase processes, including particle clustering, settling velocity, drag, and granular temperature, can be represented using physically motivated *a priori* predictors derived from high-fidelity Euler-Lagrange simulations. Collectively, these closures provide the foundation for incorporating microscale and mesoscale particle/fluid dynamics into coarse-grained multiphase flow solvers. However, an important open question remains regarding the generality of these relationships outside the parameter space investigated in this work. The simulations considered in this dissertation were intentionally limited to two particle volume fractions and two lognormal particle size

distributions to isolate the effects of polydispersity while maintaining a computationally feasible parameter space. Consequently, although the proposed functional forms successfully capture the observed behavior, many of the associated coefficients were calibrated only for the configurations investigated.

6.2.2 GENERALIZATION OF PROPOSED CLOSURE RELATIONSHIPS

The proposed *a priori* predictor for the degree of clustering (refer to (3.7)) is dependent on coefficients $\mathbb{E}$, $\mathbb{F}$, and $\mathbb{G}$ as linear functions of particle volume fraction because only two values of $\langle \alpha_p \rangle$ were available. Whether these relationships remain linear, become nonlinear, or depend additionally on particle size distribution remains unknown.

Likewise, the fluid velocity closure (refer to (3.13)) currently requires separate values of the constant coefficient $\mathbb{J}$ for each particle volume fraction considered, while the drag (refer to (3.18)) and granular temperature (refer to (5.5)) closures require independent sets of fitted coefficients for each particle size distribution and particle volume fraction.

Although these coefficients accurately reproduce the simulation data, they cannot presently be generalized to other particle-laden systems.

A natural continuation of this work is therefore to expand the simulation parameter space to include additional particle volume fractions, particle size distributions, particle density ratios, and fluid properties. Such a study would enable the development of generalized coefficient relationships that vary continuously with physically meaningful

parameters, allowing the proposed closures to be applied to other polydisperse particle-laden systems without case-by-case calibration.

6.2.3 IMPLEMENTATION WITHIN COARSE-GRAINED SOLVERS

Once generalized coefficient relationships have been established, the next stage of research will focus on implementing the proposed closures within coarse-grained Euler-Euler and Reynolds-averaged multiphase flow solvers. This will provide the first opportunity to evaluate how accurately the closures reproduce large-scale particle clustering, settling, and turbulence statistics in simulations that cannot practically be performed using high-fidelity Euler-Lagrange methods. Such validation will also identify which unresolved processes contribute most significantly to prediction error, thereby guiding future refinement of the closure models.

6.2.4 EXTENSION TO OTHER MULTIPHASE FLOWS

Future work should therefore investigate the applicability of the proposed closures to other gas-solid systems. Such studies would determine the degree to which the proposed *a priori* predictors remain universal and identify additional physical parameters that may be required for broader applicability. Establishing a generalized closure framework applicable across multiple classes of particle-laden flows would significantly improve the predictive capability of coarse-grained multiphase flow solvers used in both industrial and environmental applications.

6.3 IMPLICATIONS OF PARTICLE SHAPE AND SURFACE ROUGHNESS ON POLYDISPERSE MULTIPHASE FLOW BEHAVIOR

This dissertation treated particles as solid and spherical with uniform properties. A collision model was leveraged with a constant coefficient of elasticity. PDC particles are over various shapes, sizes, material properties, and surface roughness. It is postulated that differing volcanic material will have different coefficients of elasticity for modeling collisions. To address this gap, the Euler-Lagrange framework used in this study can be extended to other shapes, such as ellipsoids or polyhedral particles. This could be done by employing a lognormal or normal distribution defining differing particle properties. Several studies have investigated how differing surface roughness and shape affect multiphase behavior [219–224]. This topic generated several follow-up questions.

A first open question is whether the surface loading parameter, S , remains an effective *a priori* predictor when particle surface area and projected area depend on both shape and orientation. For spherical particles, particle diameter provides a direct measure of surface area. For nonspherical particles, however, equivalent diameter alone may not adequately describe the area exposed to the carrier phase. Future work could therefore examine whether S must be extended to include additional shape descriptors, such as sphericity, aspect ratio, projected-area ratio, or a characteristic surface-area-to-volume ratio.

Particle shape may also change the formation and structure of clusters.

Nonspherical particles experience orientation-dependent drag and may rotate or align with the surrounding flow, producing settling trajectories that differ from those of spheres.

These effects could modify preferential concentration, cluster compactness, fragmentation, and the rate at which clusters form. A new study could determine whether the proposed *a priori* predictor for the degree of clustering (refer to (3.7)) retains the same functional dependence on surface loading or whether additional shape-dependent parameters are required.

The proposed drag closure (refer to (3.18)) is also likely to be directly affected.

Irregular particles generally experience different drag forces than spheres because their projected area and wake behavior vary with orientation. Consequently, the coefficients in the proposed drag relationship may no longer remain valid, and the stochastic contribution may change in the presence of nonspherical particles. Future simulations could quantify these effects and develop a generalized drag closure that includes differing particle shapes, sizes, and surface roughness.

Finally, surface roughness may affect collision statistics by modifying the coefficient of restitution, friction, and contact duration. These changes could influence collision frequency, cluster breakup, and the balance between particle-phase kinetic energy and granular temperature. A follow-up study would therefore require coordinated changes to the particle-collision model.

APPENDIX A
DISTRIBUTION TERMINOLOGY

While the applications of polydisperse gas-solid flows are far-reaching, ranging from natural to industrial flows, the parameters under study in this work are drawn from PDCs. In the geoscience community, it is common to quantify the distribution of sedimentary particles using a convention referred to as the ‘ ϕ scale.’ Since this convention is less common in other areas of science and the applications of this study are far reaching outside the geoscience community, we present here a very brief discussion connecting the ϕ scale with a standard log-normal distribution defined in terms of millimeters.

As such, the ϕ scale was developed on the notion that sediment behavior is a function of particle diameter squared. Thus, $\phi \equiv -\log_2(d_p)$ is used as the basis for this scale[225]. It is important to note that in the definition of ϕ the particle diameter, d_p , has units of millimeters. Since the basis of ϕ definition is $\log_2$, then the parameter $\phi_{\text{textsorting}}$ describes the *normal* distribution of the particles in terms of ϕ . This also implies that the distribution of particle diameter in units of mm is log-normal.

To traverse these two definitions for particle distribution, one can make use of the following relationships:

$$\langle d_p \rangle = 2^{-\phi} \quad (\text{A.1})$$

$$\mu = \ln(\langle d_p \rangle) = \ln(2^{-\phi}) \quad (\text{A.2})$$

$$\sigma = \phi_{\text{sorting}}^2 \ln(2)^2 \quad (\text{A.3})$$

where $\langle d_p \rangle$ represents the mean particle diameter in millimeters and μ and σ represent the standard log-normal parameters, such that the probability distribution function for particle diameter is defined as

$$f_{d_p} = \frac{1}{d_p \sigma \sqrt{2\pi}} \exp \left(-\frac{(\ln d_p - \mu)^2}{2\sigma^2} \right) \quad (\text{A.4})$$

APPENDIX B
STATISTICAL DIAMETERS

When considering assemblies of particles of varying size, as is done in this work, it is often informative to quantify how particles are distributed by using the following statistical diameters:

1. D_{10} represents the mean diameter in the usual, arithmetic sense as

$$D_{10} = \frac{\sum_{i=1}^{N_p} d_p^{(i)}}{N_p} \quad (\text{B.1})$$

2. D_{20} represents the surface mean diameter. In other words, this is diameter of a monodisperse assembly of N_p particles with the same total surface area of the polydisperse assembly. It is defined as

$$D_{20} = \sqrt{\frac{\sum_{i=1}^{N_p} (d_p^{(i)})^2}{N_p}} \quad (\text{B.2})$$

3. D_{30} represents the volume mean diameter. Similar to the surface mean diameter, this value represents the diameter of a monodisperse assembly of N_p particles with the same total volume as the polydisperse assembly. It is given as

$$D_{30} = \left(\frac{\sum_{i=1}^{N_p} (d_p^{(i)})^3}{N_p} \right)^{1/3} \quad (\text{B.3})$$

4. D_{32} denotes the surface moment mean diameter, commonly referred to as the Sauter mean diameter. This is the diameter required for a monodisperse assembly of N_p particles to have the same ratio of volume to surface area as the polydisperse assembly.

$$D_{32} = \frac{\sum_{i=1}^{N_p} (d_p^{(i)})^3}{\sum_{i=1}^{N_p} (d_p^{(i)})^2} = \frac{D_{30}^3}{D_{20}^2} \quad (\text{B.4})$$

5. D_{43} denotes the volume moment mean diameter. This quantity is an indicator of which particle sizes contain a majority of the particle volume.

$$D_{43} = \frac{\sum_{i=1}^{N_p} (d_p^{(i)})^4}{\sum_{i=1}^{N_p} (d_p^{(i)})^3} \quad (\text{B.5})$$

APPENDIX C
SHORT LIST OF VARIABLES

Table 3.1: List of Variables

<i>Symbol</i>	<i>Variable</i>	<i>Units</i>
μ	log-normal shape parameter	
σ	log-normal shape parameter	
ϕ	phi scale diameter distribution	
ϕ_{sorting}	sorting parameter	
α	fluid phase volume fraction	
α_p	particle phase volume fraction	
$\langle \alpha_p \rangle$	particle volume fraction	
α_{rcp}	random closed packing volume fraction	
φ_0	<i>a priori</i> mass loading	
$\mathcal{S}$	surface loading	
$\mathcal{D}$	degree of clustering	
N_p	number of particles	
ρ_p	particle density	[kg/m ³]
ρ_f	fluid density	[kg/m ³]
ν_f	fluid dynamic viscosity	[kg/(ms)]
μ_f	fluid kinematic viscosity	[m/s ²]
C_D	gas-particle drag coefficient	
F_D	drag correction	
$\mathbf{g}$	gravity	[m/s ²]
$d_{\min}$	minimum particle diameter	[mm]
$d_{\max}$	maximum particle diameter	[mm]
$\langle d_p \rangle$	mean particle diameter	[mm]
$\sqrt{\langle d_p'^2 \rangle}$	standard deviation	[mm]
D_{10}	mean diameter	[mm]
D_{20}	surface mean diameter	[mm]
D_{30}	volume mean diameter	[mm]
D_{32}	surface moment mean diameter	[mm]
D_{43}	volume moment mean diameter	[mm]
$\tau_{p,10}$	particle relaxation time	[s]
$\tau_{p,20}$	particle relaxation time	[s]
$\tau_{p,30}$	particle relaxation time	[s]
$\tau_{p,32}$	particle relaxation time	[s]
$\tau_{p,43}$	particle relaxation time	[s]
$\mathcal{V}_{\min}$	Stokes settling velocity	[m/s]
$\mathcal{V}_{0,10}$	Stokes settling velocity	[m/s]
$\mathcal{V}_{0,20}$	Stokes settling velocity	[m/s]
$\mathcal{V}_{0,30}$	Stokes settling velocity	[m/s]
$\mathcal{V}_{0,32}$	Stokes settling velocity	[m/s]

<i>Symbol</i>	<i>Variable</i>	<i>Units</i>
$\mathcal{V}_{0,43}$	Stokes settling velocity	[m/s]
$\mathcal{V}_{0,max}$	Stokes settling velocity	[m/s]
$\mathcal{V}_s$	depth-averaged settling velocity	[m/s]
$\text{Re}_{p,10}$	particle Reynolds number	
$\text{Re}_{p,32}$	particle Reynolds number	
Fr_{10}	Froude number	
Fr_{32}	Froude number	
δ^*	normalized filter size	
$n_x \times n_y \times n_z$	computational grid	
$L_x \times L_y \times L_z$	domain size	[mm]

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