Application of Discrete Element Method and Computational Fluid Dynamics to Selected Dispersed Phase Flow Problems

Oladapo Olanrewaju Ayeni
Louisiana State University and Agricultural and Mechanical College, oayeni1@lsu.edu

Follow this and additional works at: https://digitalcommons.lsu.edu/gradschool_dissertations
Part of the Chemical Engineering Commons

Recommended Citation
https://digitalcommons.lsu.edu/gradschool_dissertations/3069

This Dissertation is brought to you for free and open access by the Graduate School at LSU Digital Commons. It has been accepted for inclusion in LSU Doctoral Dissertations by an authorized graduate school editor of LSU Digital Commons. For more information, please contact gradetd@lsu.edu.
APPLICATION OF DISCRETE ELEMENT METHOD AND COMPUTATIONAL FLUID DYNAMICS TO SELECTED DISPERSED PHASE FLOW PROBLEMS

A Dissertation

Submitted to the Graduate Faculty of the Louisiana State University and Agricultural and Mechanical College in partial fulfillment of the requirements for the degree of Doctor of Philosophy

in

The Gordon A. and Mary Cain Department of Chemical Engineering

by

Oladapo Olanrewaju Ayeni
B.S., University of Lagos, 2006
M.S., Louisiana State University, August, 2013
December 2015
Acknowledgements

First, I would like to thank my advisor, Professor Krishnaswamy Nandakumar for his tireless guidance throughout my doctorate program and having more confidence in my ability to complete this program than I had in myself.

I would like to thank Professor J. B. Joshi for co-advising my project and investing his time and wealth of experience in the field of multiphase flow research to guiding me through some of the more important problems in the field deserving of attention.

I would be remiss to mention Dr. Chunliang Wu who not only granted me full permissions to his Discrete Particle Model code but also was actively involved in every area of my research including publications, presentations and this dissertation. Without his mentorship, this project would never have been completed.

I would like to pay courtesy to past and present members of the EPIC research consortium including post-doctoral fellows Drs. Mayur Saathe, Shivkumar Bale, Yuehao Li and fellow graduate students Abhijit, Gongqiang, Chenguang, Aaron, LC, Jielin, Daniel and John.

Finally, I would like to dedicate this dissertation to my parents, Dr. and Mrs. Oladapo Ayeni and my four sisters, Oluwatosin, Oluwatoyosi, Aanuoluwakitan and Oluwabusola. I would not have made it this far in life without your unconditional love.

A dream fulfilled is a tree of life – Proverbs 13:12
# Table of Contents

Acknowledgements................................................................................................. ii

List of Tables .......................................................................................................... v

List of Figures .......................................................................................................... vi

Notation .................................................................................................................... xi

Abstract.................................................................................................................. xiv

Chapter 1 General Introduction........................................................................... 1

Chapter 2 Analytical and Computational Considerations for Particulate Flow Modeling........................................................................................................ 6
  2.1 Volume Averaging ............................................................................................... 6
  2.2 Model A and B .................................................................................................. 11
  2.3 Particle dynamics ............................................................................................. 12
    2.3.1 Hard-sphere model .................................................................................... 14
    2.3.2 Soft-sphere model .................................................................................... 16
  2.4 Discretization of the volume-averaged equations for a flow solver ............. 20
  2.5 Source terms and numerical stability ............................................................. 23
  2.6 Discretization of particle dynamic equations ................................................... 24
  2.7 Implementation of Source Terms In Fluent .................................................... 25
  2.8 Parallel computing considerations ................................................................. 27

Chapter 3 Behavior of Clusters of Particles in a Viscous Ambient Fluid............ 29
  3.1 Introduction ..................................................................................................... 29
  3.2 Literature review ............................................................................................ 32
    3.2.1 Phases of cloud settling .......................................................................... 44
    3.2.2 Velocity fluctuation ................................................................................ 45
    3.2.3 Particle clouds and immiscible liquid drops and their similarities ......... 47
  3.3 Computational setup ....................................................................................... 48
    3.3.1 Two-way coupling .................................................................................. 48
    3.3.2 Initial and boundary conditions ............................................................... 49
  3.4 Results and discussion ................................................................................. 49
    3.4.1 Validation .................................................................................................. 49
    3.4.2 Particle leakage at low \(Re_c\) .................................................................. 54
    3.4.3 Breakup At moderate \(Re_c\) .................................................................. 56
    3.4.4 Interaction among multiple drops ........................................................... 68
  3.5 Conclusions .................................................................................................... 75

Chapter 4 Simulation of Gas-Solid Flows in a Small-Scale Fluidized Bed Using a Newly Developed Momentum Interphase Drag Coefficient ..................................................... 77
  4.1 Introduction ..................................................................................................... 77
  4.2 Simulation method ......................................................................................... 79
  4.3 Closure models ............................................................................................... 79
    4.3.1 New drag model ...................................................................................... 80
  4.4 Results ............................................................................................................ 84
  4.5 Conclusions .................................................................................................... 96
List of Tables

Table 3-1: Summary of research in particle cloud settling ................................................................. 44

Table 3-2: Comparison of $Nc$ dependence of settling speed in theory and simulations.......................... 51

Table 3-3: Parameters for the Particle number parameter study ................................................................ 55

Table 3-4: Comparison of break up quantities of and initially random cloud configuration and non-
random configuration of particles ........................................................................................................ 60

Table 3-5: Observed critical aspect ratio for particle cloud settling ......................................................... 63

Table 4-1: Computation Parameters ...................................................................................................... 84

Table 5-1: Parameters used in the validation of the DEM code............................................................... 107
List of Figures

Figure 1-1: Illustration of regime change in particle-fluid systems .................................................. 3

Figure 1-2: Illustration of Hierarchy of modeling from sub-atomic models to phenomenological mixture
models ........................................................................................................................................... 4

Figure 2-1: Control Volume in a multiphase system (link) ................................................................. 6

Figure 2-2: Hard-Sphere Model Calculation Sequence ................................................................. 14

Figure 2-3: Illustration of Binary Collision .................................................................................. 14

Figure 2-4: Soft-Sphere Model Illustration .................................................................................. 17

Figure 2-5: Solution Algorithm Flow Chart ............................................................................... 27

Figure 2-6: Parallel Speedup for increasing number of cores ...................................................... 28

Figure 3-1: Homogeneous (left) and inhomogeneous (right) dispersions .................................... 31

Figure 3-2: Three regimes of cloud settling based on particle and cloud scale inertia 26 .......... 37

Figure 3-3: Open torus showing fluid streamlines passing through the center. Only particles in the
meridian plane are shown for clarity .............................................................................................. 38

Figure 3-4: Stream Envelope at low Re ..................................................................................... 41

Figure 3-5: (A) Steady-state settling velocity vs Npe; (B) Settling Velocity dependence on volume
fraction ........................................................................................................................................... 51

Figure 3-6: (A) Vertical velocity fluctuations with volume fraction dependence (B) Horizontal velocity
fluctuations with volume fraction dependence ............................................................................ 51

Figure 3-7: (A) Evolution of Scaled cloud settling velocity with scaled time at Rec = 11.4 (B) Evolution
of Cloud aspect ratio with scaled time at Rec = 11.4 ................................................................. 52

Figure 3-8: Evolution of scaled cloud settling velocity with scaled time at Rec = 14 (B) Evolution of
cloud aspect ratio with scaled time at Rec = 14 ........................................................................ 53

Figure 3-9: Particle leakage at low Reynolds Number ................................................................. 54

Figure 3-10: Particle Leakage with time for various initial number of particles ............................ 56

Figure 3-11: Rate of particle leakage with initial number of particles .......................................... 56
Figure 3-12: Comparison between breakup into secondary drops ni experiments (left) and simulation (right) at \( \text{Rec} = 5.0 \) .................................................................57

Figure 3-13: Effect of nature and shape of boundaries on breakup pattern showing top (top) and side view (bottom) ..............................................................58

Figure 3-14: Effect of Nature of boundaries on velocity fluctuations in (A) Vertical and (B) Horizontal directions........................................................................59

Figure 3-15: Breakup pattern for (A) an initially random (B) Non-random particle distribution........60

Figure 3-16: Comparison of Cloud evolution for initially random and non-random particle distributions (A) Aspect ratio evolution (B) Velocity auto-correlation function evolution.................................60

Figure 3-17: Schematic showing evolution of the cloud aspect ratio before and after the point of breakup .................................................................62

Figure 3-18: Aspect ratio evolution with time at different Reynolds number .........................62

Figure 3-19: Effect of \( \text{Rec} \) on (A) breakup time; (B) breakup length........................................63

Figure 3-20: Normalized average settling velocity of cloud vs. normalized time for different Reynolds numbers........................................................................65

Figure 3-21: Scaled velocity auto-correlation function with time at different \( \text{Rec} \) .................66

Figure 3-22: Velocity Auto-correlation function at \( \text{Rec} = 0.1 \) ..............................................66

Figure 3-23: Shape evolution at \( \text{Rec} = 0.1 \) ......................................................................67

Figure 3-24: Shape evolution at \( \text{Rec} = 1.0 \) ..................................................................67

Figure 3-25: Shape evolution at \( \text{Rec} = 2.0 \) ..................................................................67

Figure 3-26: Shape evolution at \( \text{Rec} = 5.0 \) ..................................................................67

Figure 3-27: Shape evolution at \( \text{Rec} = 10.0 \) .................................................................68

Figure 3-28: Shape evolution at \( \text{Rec} = 50.0 \) .................................................................68

Figure 3-29: Pressure and velocity field evolution of 2 descending, coaxially initialized clouds ..........69

Figure 3-30: Comparison between two trailing buoyant drops of different radiuses and two trailing particle clouds of different radiuses in coaxial positions........................................70

Figure 3-31: Comparison between two trailing drops of different radiuses and two particle clouds of different radiuses in off-symmetry positions ..................70
Figure 3-32: Comparison between two trailing drops of different radiiuses and two trailing particle clouds of different radiiuses in accentuated off-symmetry positions ................................................................. 70

Figure 3-33: Structure evolution of two particle clusters – Heavy Leading, Light Trailing. Top line graph is RMS in x-direction while bottom is skewness in y-direction ......................................................... 72

Figure 3-34: Enhancement of vertical velocity of trailing, light cluster ............................................. 73

Figure 3-35: Structure evolution of two particle clusters – Heavy Trailing, Light Leading Top line graph is RMS in x-direction while bottom is skewness in y-direction ......................................................... 74

Figure 3-36: Enhancement of velocity of trailing, Heavy cluster ....................................................... 75

Figure 4-1: Geometry for the fluidized bed ....................................................................................... 83

Figure 4-2: Complex bubbling-slugging regime at inlet velocity of 2umf ........................................ 86

Figure 4-3: Time-averaged horizontal solid velocity profile at inlet velocity of 2umf for the 3 drag models used ................................................................................................................................. 87

Figure 4-4: Time-averaged vertical solid velocity profile at inlet velocity of 2umf for the 3 drag models used ................................................................................................................................. 87

Figure 4-5: Complex bubbling-slugging regime at inlet velocity of 3umf ........................................ 88

Figure 4-6: Time-averaged horizontal solid velocity profile at inlet velocity of 3umf for the 3 drag models used ................................................................................................................................. 89

Figure 4-7: Time-averaged horizontal solid velocity profile at inlet velocity of 3umf for the 3 drag models used ................................................................................................................................. 89

Figure 4-8: Complex bubbling-slugging regime at inlet velocity of 4umf ........................................ 90

Figure 4-9: Time-averaged horizontal solid velocity profile at inlet velocity of 4umf for the 3 drag models used ................................................................................................................................. 91

Figure 4-10: Time-averaged horizontal solid velocity profile at inlet velocity of 4u_mffor the 3 drag models used ................................................................................................................................. 91

Figure 4-11: Time-averaged axial pressure drop between z=0.0413m and 0.3641m. Curve 1 uses Gidaspow, 2 uses Syamlal, 3 uses the new drag law and 4 corresponds to experiments ........................................ 92

Figure 4-12: RMS axial pressure drop between z=0.0413m and 0.3641m. Curve 1 uses Gidaspow, 2 uses Syamlal, 3 uses the new drag law and 4 corresponds to experiments ........................................ 93

Figure 4-13: Time-series and Fourier transform of the pressure drop signal for the simulated cases and experiments ................................................................................................................................. 94
Figure 4-14: Time-averaged transverse vertical solid velocity profile at z=0.076m. 1 is using Gidaspow, 2 Syamlal, 3 the new drag law.

Figure 4-15: Axial solid holdup profile for 3 inlet flow rates predicted by Gidaspow (curve 1), Syamlal (curve 2) and the current drag law (curve 3).

Figure 5-1: Rolling (Avalanche) Regime. Fr=0.002686
Figure 5-2: Cataracting Regime, Fr=0.7339
Figure 5-3: Centrifuging Regime, Fr=4.5872
Figure 5-4: Comparison Between pattern formation in rotating tumbler in simulations and experiments.
Figure 5-5: Segregation of particles in a square tumbler
Figure 5-6: Segregation and streaking of a mixture of steel particles (red, 1mm) and glass beads (blue, 2mm) in a square tumbler comparison to Jain, Ottino and Lueptow.
Figure 5-7: Time evolution area-based segregation intensity for simulation(red line with star) and experiments Jain, Ottino and Lueptow (blue cross): (A) “D” system with 4mm steel balls and 4mm glass balls; (B) “S+D” system with 3mm steel balls and 4mm glass balls; (C) “S+D” system with 1mm steel balls and 2mm glass balls.
Figure 5-8: Schematic to illustrate coordination number fraction
Figure 5-9: Various computation domains used in the simulations
Figure 5-10: Particle distribution after 20 revs in various shaped tumblers. The first row is for a elliptical tumblers at ½ fill while second row is for rectangular tumblers at ½ fill. The displacement of the core of particles towards the left is due to the direct...
Figure 5-11: Velocity Field of a circular tumbler at ¼ fill.
Figure 5-12: (A) Particle trajectories in circular tumbler for small steel particles (red) and large glass beads (blue) (B) Radial segregation in tumbler.
Figure 5-13: Particle Trajectory in tumbler e2 with an aspect ratio equal to 2.25
Figure 5-14: Evolution of mixing entropy for various tumblers (A) For tumblers e0, e1 and e2 at ¼ fill, (B) For tumblers e0, e1 and e2 at ½ fill
Figure 5-15: Evolution of mixing entropy for various tumblers (A) For tumblers r0, r1 and r2 at ¼ fill, (B) For tumblers r0, r1 and r2 at ½ fill.
Figure 5-16: Frequency spectrum in (A) tumbler e1 at ¼ fill, (B) tumbler e1 at ½ fill, (C) tumbler e2 at ¼ fill, (D) tumbler e2 at ½ fill.

Figure 5-17: Motion of the centroid of the core of steel particles beginning at the filled circle and terminating at the star.

Figure 5-18: Frequency spectrum in (A) tumbler r1 at ¼ fill, (B) tumbler r1 at ½ fill, (C) tumbler r2 at ¼ fill, (D) tumbler r2 at ½ fill.

Figure B-1: Comparison between $3.6e6G4 + 1$ and $e - 4.8$.

Figure B-2: Comparison between equation (B44) and (B45).
Notation

Chapter 2
Symbols
\( V \) – Volume (m\(^3\))
\( v \) – Velocity, (m/s)
\( X \) – Body force per unit mass, (m/s\(^2\))
\( A \) – Area (m\(^2\))
\( n \) – Unit normal
\( t \) – Unit tangent
\( \dot{m} \) – Mass transfer rate per unit volume (kg/s-m\(^3\))
\( m \) – Mass of particle (kg)
\( S \) – Source term (N/m\(^3\))
\( S \) – Mass source (kg/s-m\(^3\))
\( K \) – Interphase momentum coefficient (kg/s-m\(^3\))
\( g \) – Acceleration due to gravity (m/s\(^2\))
\( p \) – Pressure (Pa)
\( F \) – Contact forces (N)
\( R \) – Particle radius (m)
\( G \) – Relative translational velocity (m/s)
\( e \) – Restitution coefficient
\( k \) – Spring constant
\( E \) – Young’s modulus
\( d \) – Diameter (m)
\( \pi \) – Number of phases
\( \varepsilon \) – Volume fraction
\( \Phi, \Psi \) – Arbitrary properties
\( \rho \) – Density (kg/m\(^3\))
\( \sigma \) – Total stress (Pa)
\( \beta \) – Interphase momentum transfer coefficient (kg/s-m\(^3\))
\( \omega \) – Rotational velocity (rad/s)
\( \delta \) – Overlap (m)
\( \vartheta \) – Poisson ratio
\( \eta \) – Damping coefficient
\( \tau \) – Shear stress (N/m\(^2\))
\( \tau \) – Fluid response time (s)
\( \Gamma \) – Property diffusivity

Subscripts
\( j, k \) – Phase index
\( l \) – Phase index for phase other than current phase
\( s \) – Solid phase
\( n \) – Normal
\( t \) – Tangential
\( p \) – Particle phase

Chapter 3
Symbols
\( u_s \) – Settling Velocity of Suspension (m/s)
\( u_0 \) – Terminal settling velocity of single particle (m/s)
φ – Solids volume fraction
\( G, \psi \) – Arbitrary quantity
\( x \) – Position vector (m)
\( P \) – Probability distribution
\( \mathcal{G} \) – Particle configuration
\( N \) – Number of particles
\( \epsilon \) – Ratio of particle radius to cloud radius
\( R \) – Radius of cloud (m)
\( a \) – Radius of particle (m)
\( d \) – Mean particle spacing (m)
\( Re \) – Reynolds number
\( \rho \) – Density (kg/m\(^3\))
\( g \) – Acceleration due to gravity (m/s\(^2\))
\( \mu \) – Dynamic viscosity (Pa-s)
\( St \) – Stokes number
\( l \) – Inertial length (m)
\( Fr \) – Froude number
\( \xi \) – Correlation length (m)
\( V \) – Volume (m\(^3\))
\( n \) – Number density of particles
\( \beta \) – Interphase momentum coefficient (N/m\(^4\))
\( C_D \) – Drag coefficient
\( \nu \) – Volume fraction of continuous phase
\( k \) – Spring constant
\( e \) – Restitution coefficient
\( \omega \) – Angular velocity (rad/s)
\( \eta \) – Damping coefficient

**Subscripts**
\( s \) – Solids
\( N \) – Number of particles
\( c \) – Cloud
\( p \) – Particle
\( k \) – Index
\( \tau \) – Particle response time
\( S \) – Momentum source
\( m \) – Mass
\( n \) – Normal
\( t \) – Tangential
\( \gamma \) – Aspect ratio
\( b \) – Breakup

**Superscripts**
\( ^* \) – Normalized quantity

**Abbreviations**
DPM – Discrete Particle Model
VACF – Velocity Auto-Correlation Function

**Chapter 4**
**Symbol**
\( Fr \) – Froude number
\( d \) – Diameter (m)
\( C_D \) – Coefficient of drag
\( Re \) – Reynolds number
$K$ – Drag adjustment factor
$\varepsilon$ – Voidage
$\mu$ – Dynamic viscosity (kg/m-s)
$\rho$ – Density
$\beta$ – Momentum interphase coefficient (kg/s-m$^3$)

**Subscript**
$m_f$ – Condition at minimum fluidization
$p$ – Particle
$s$ – Solid

**Chapter 5**
**Symbols**
$p$ – Coordination fraction
$C_n$ – Coordination number
$r$ – Particle radius
$N_p$ – Number of particles
$S$ – Mixing entropy
$\gamma$ – Tumbler aspect ratio
Abstract

A parallel discrete particle modelling framework (PAR_DPM3D) is applied to study three fundamental multiphase flow problems: The sedimentation of a cluster of particles in a viscous ambient fluid, multiphase flow in a bench-scale fluidized bed and granular segregation and mixing dynamics in a rotating drum.

Various phenomena including torus formation and particle cluster breakup are reproduced. We provide new insights into the volume fraction dependence of the dynamic characteristics of a settling particle cluster and find a similar dependence in the simulations as in the theoretical predictions of Nitsche and Batchelor \(^1\). Similarities in the interaction between a system of two particle clouds and a system of two immiscible droplets was established with an observed increase in the velocity of the trailing cloud due to drag reduction in the wake of the leading cloud.

Second, we show how existing drag models may be inadequate to predicting the macroscale properties of a gas-solid fluidized bed. Using an energy and force balance approach we provide new closures that account for some inhomogeneous flow structures and implement these closures within the PAR_DPM3D framework to predicting the axial pressure drop and transverse particle velocity profiles.

Finally, we present results from particle dynamics simulation of “S+D” granular systems (where size and density drive segregation simultaneously) in various irregular shaped tumblers in the rolling regime \((10^{-4} < Fr < 10^{-2})\). We develop a new way of quantifying the state of mixing or segregation. Using this new measure of segregation (or entropy of mixing) we compare segregation dynamics for different shapes of tumblers.
Chapter 1 General Introduction

Multiphase flow is the simultaneous flow of two or more constituents and covers a wide variety of flow scenarios within continuum mechanics. It is distinct from multicomponent flows. A multicomponent system is one in which there is a material connection among the constituents of a fluid. For instance, air which is a mixture of various component gas represents such a system. Material connection often means that considerable effort is required in separating out the components since they are homogeneously mixed over very large length scales. However, in a multiphase system, there is no clear material connection between the various constituent parts of the system. For instance, while steam bubbles existing alongside liquid water at the dew point may have the same chemical makeup, it is easy to make out with the naked eye the interface that separates the vapor from the liquid. Using a simple gravity-driven separator, a steam and water can be separated whereas the separation of nitrogen from oxygen in air may require more involved complex membrane or cryogenic separators.

As an additional example, the flow of water with oil, both existing in a liquid state would can be termed a multiphase mixture since both are immiscible. Hence the analysis of such a flow is best described by models that take into account the physical properties that include density and viscosity of both the continuous and the dispersed phase separately.

According to Crowe multiphase flows are divided into no less than four broad categories: gas-solid, gas-solid, liquid-solid and three phase flows. A definition of which phase is the dispersed phase and which is the continuous phase is increases the number of classifications. For instance, the sparging of gas into a bubble column may represent a type of gas-liquid flows where the gas is the dispersed phase and the liquid is the continuous phase, whereas, the counter current flow of
liquid drops and gas in a spray-dryer is another type of liquid-gas flows where the dispersed phase is the liquid and the continuous phase is the gas. This subtle difference may offer profound differences in the way the multiphase model relationships are posed. Also notable is the convention in naming such multiphase systems where the dispersed phase is called first and the continuous phase is called second \(^3\) an example being again the bubble column which would be appropriately termed a gas-liquid system while a spray dryer will be called a liquid-gas system.

For many years our observation of multiphase systems has been guided by empiricism with very little fundamental information being provided on very simple systems. For instance the solution of the drag across a single particle in creeping flow has been calculated analytically many years ago by Stokes \(^4\) whereas the drag in a fixed bed of particles with a random configuration has been determined empirically by making connections to averaged macroscale quantities such as the volume fraction of particles and pressure drop across the bed \(^5\). However, with the increase in computational capability and sophisticated computational modelling, it is possible to determine the hydrodynamics of multiphase systems without resorting to ad-hoc, empirical, bench-scale observations which may not scale up industrially. This provides immense benefits in process design, control, optimization and intensification.

As can be seen in figure 1-1, there is a variety of multiphase flow scenarios in the simultaneous flow of gas and solid and unique computational methods exist for the simulation of these. Dependent upon the flow of fluid into the domain through the inlet of the vessel, the flow could be particulate [as with solid-liquid fluidization], aggregative [as with gas-solid fluidization] or if the flow rate of gas is high enough result in pneumatic conveying of particles.
This work is concerned with dispersed phase, solid-liquid or solid-gas flows where solid particles form the dispersed phase.

In modelling solid-fluid flows in general, considerations have to be made regarding the approach we intend to employ. Depending on the computational resources at hand, simulation of physical systems span the entire spectrum of physics that can be simulated. Figure 1-2 provides a rough picture of the various levels and approaches of modeling from large scale phenomenological models to sub-atomic scale ab-initio methods depending on solutions to Schrödinger wave equation. The picture is clear in that none of these models exist in isolation and often, the length and time scales determine the amount of closures that are required to use a particular model.

Of particular interest to us in this work is the orange highlighted box, the Discrete Element Model (DEM) which is a special class of Discrete Particle Methods (DPM) which we apply to solve certain interesting Eulerian-Lagrangian (E-L) dispersed phase flow problems.
With reference to particulate systems in the chemical process industry, we identified three areas of fluid-particle multiphase flow. In systems that involve pneumatic conveyor, solid-liquid flows are predominant. Examples of these include the transport of drill cuttings from a well-bore or proppant into a fracture in oil production. The second area of fluid-particle interactions we identify would be gas-solid interactions. Processes that require an understanding of this field include coal gasification, fluid-catalytic cracking processes and cyclone separation. The third area we identify are systems where particle-particle interactions dominate over particle fluid interactions. For all intents, fluid flow can be neglected in the dynamics of the system in favor of dissipative collisions. Examples of equipment that benefit from an improved knowledge of the underlying science of granular flows include rotary kilns, grain silos and mixing equipment. It is the goal of this work to show that a conceptually simple framework such as the Euler-Lagrange (E-L) approach can capture many complex mesoscale flow features including particle clustering, bubble-formation, mixing and segregation patterns in granular systems. These areas have been selected to reflect phenomena liquid-solid systems, gas-solid systems and dense particulate systems.
In chapter 2 we give a brief description of the origin of mesoscale models and the concept of phase-averaging and relate it to E-L governing equations. We also describe in brief details about the flow solver we employ throughout the work and the hybrid parallelization scheme used to speed up calculation.

In chapter 3 we present results of the application of E-L methods to studying the behavior of a swarm of particles in a viscous liquid under the action of gravity and show different flow patterns.

In chapter 4, we apply the E-L equations to a laboratory scale gas-solid fluidized bed and show why pressure drop as well as transverse velocity profile in such beds may often be over-predicted using available drag closures. We make an attempt to address this concern by mechanical energy balance analysis.

In chapter 5, we study the segregation and mixing in circular and non-circular rotating drums where Knudsen number is highest among cases we studied. We show the segregation and mixing patterns for different particle mixtures and show how the dynamics of segregation and mixing can be greatly altered by microscopic quantities like density and size differences and macroscopic quantities such as the shape of the vessel.

A summary of the of the major contributions of this study will be presented in Chapter 6 and we will offer concluding thoughts about some open questions in the application of discrete element methods to improving our understanding of multiphase flows.
Chapter 2 Analytical and Computational Considerations for Particulate Flow Modeling

Particulate flows fall under the general area of dispersed phase flows which includes gas-droplet, gas-particle and liquid-particle flows. The particles and droplets form the dispersed phase. In this section, we will present a brief derivation of the volume-averaged Navier Stokes equations and illustrate the usage of the parallel flow code, PAR-DPM3D, developed by Wu, Ayeni, Berrouk and Nandakumar to simulate large-scale particulate system and the speed-up that the hybrid parallel architecture provides.

2.1 Volume Averaging

Figure 2-1 shows an idealization of the control volume in a multiphase system with a number of subdomains corresponding to different phases within the entire volume.

![Figure 2-1: Control Volume in a multiphase system](link)

An extended form of the derivation of the volume-averaged equations can be seen here: link. We can calculate the sum of the entire control volume as a sum of all the volume of all the phases as in equation 2.1

\[ \Delta V = \sum_{k=1}^{\pi} \Delta V_k \]  

(2.1)
Where \( k \) is the index denoting the phases and \( \pi \) is the total number of phases in the control volume.

Accordingly, the volume fraction of each individual phase is given in equation 2.2

\[
\varepsilon_k = \frac{\Delta V_k}{\Delta V} \quad (2.2)
\]

Trivially, the sum of the volume fraction is 1

\[
\sum_{k=1}^{\pi} \varepsilon_k = 1 \quad (2.3)
\]

The definition of the volume average of a field property \( \Phi \) which is a function of the spatial and temporal coordinates \( x, y, z \) and \( t \) – for a multiphase system is:

\[
\langle \Phi \rangle = \frac{1}{\Delta V} \sum_{k=1}^{\pi} \int_{\Delta V_k} \Phi_k(x, y, z, t) \, dV \quad (2.4)
\]

The phase average is an intrinsic property and can be related to the volume average. It is defined for said property as follows

\[
\langle \Phi_k \rangle = \frac{1}{\Delta V_k} \int_{\Delta V_k} \Phi_k(x, y, z, t) \, dV \quad (2.5)
\]

The equivalent extrinsic average which is based on a control volume that may consist of more than one phase is:

\[
\langle \Phi_k \rangle = \frac{1}{\Delta V} \int_{\Delta V_k} \Phi_k \, dV \quad (2.6)
\]

The intrinsic and extrinsic averages are related through the volume fraction as
\[ \varepsilon_k (\Phi_k)^k = \langle \Phi_k \rangle \]  \hspace{1cm} (2.7)

Also, the volume average of the property over the entire control volume is

\[ \langle \Phi \rangle = \sum_{k=1}^{\pi} \langle \Phi_k \rangle = \sum_{k=1}^{p_i} \varepsilon_k (\Phi_k)^k \]  \hspace{1cm} (2.8)

As with the Reynolds-Averaging process, we can define “deviation” properties with the caret symbol.

\[ \hat{\Phi}_k = \Phi_k - (\Phi_k)^k \]  \hspace{1cm} (2.9)

The definition of the product of two properties follows

\[ (\Phi_k \Psi_k)^k = \varepsilon_k (\Phi_k)^k (\Psi_k)^k + \langle \hat{\Phi}_k \hat{\Psi}_k \rangle \]  \hspace{1cm} (2.10)

According to Reynolds Transport Theorem (RTT), the accumulation of a property is equal to the sum of the fluxes into the control volume. Each of the terms in the RTT can be averaged as follows:

Accumulation:

\[ \langle \frac{\partial \Omega_k}{\partial t} \rangle = \frac{\partial}{\partial t} \langle \Omega_k \rangle - \frac{1}{\Delta V} \int_{A_k} \Omega_k v_I \cdot n_k \, dA_k \]  \hspace{1cm} (2.11)

Gradient

\[ \langle \nabla \Omega_k \rangle = \nabla \langle \Omega_k \rangle + \frac{1}{\Delta V} \int_{A_k} \Omega_k n_k \, dA_k \]  \hspace{1cm} (2.12)

Laplacian:

\[ \langle \nabla \cdot \Omega_k \rangle = \nabla \cdot \langle \Omega_k \rangle + \frac{1}{\Delta V} \int_{A_k} \Omega_k \cdot n_k \, dA_k \]  \hspace{1cm} (2.13)

Using the definitions presented we perform a phase average of the continuity equation:
\[
\frac{\partial}{\partial t}(\varepsilon_k \rho^k) + \nabla \cdot (\varepsilon_k \rho^k v_k^k) = \sum_{j=1}^{\pi} \frac{m_{jk}}{m_k}
\] (2.14)

\(\rho\) is the density of the entire mixture. The term on the right hand side of equation 2.14 represent exchange of material from phase \(j\) to phase \(k\). For the momentum equation, phase averaging gives:

\[
\langle \frac{\partial \rho_k v_k}{\partial t} \rangle + \langle \nabla \cdot (\rho_k v_k v_k) \rangle = \langle \nabla \cdot \sigma'_k \rangle + \langle \rho_k X_k \rangle
\] (2.15)

\(\sigma\) is the total stress in the phase and \(X_k\) is the net body force on the phase. Using the definitions from the RTT for the gradient, laplacian and partial derivative terms, we get

\[
\frac{\partial \langle \rho_k v_k \rangle}{\partial t} + \nabla \cdot (\langle \rho_k v_k v_k \rangle)
\]

\[
= \nabla \cdot (\langle \sigma'_k \rangle) - \frac{1}{\Delta V} \int_{A_k} \rho_k (v_k v_l - v_k v_k) \cdot n_k dA_k
\]

\[
+ \frac{1}{\Delta V} \int_{A_k} \sigma'_k \cdot n_k dA_k + \langle \rho_k \rangle X_k
\]

We can now substitute for quantities in terms of average and deviation quantities and ignore product of deviations.

\[
\frac{\partial}{\partial t}(\varepsilon_k (\rho_k)^k (v_k)^k) + \nabla \cdot (\varepsilon_k (\rho_k)^k (v_k)^k (v_k)^k) = \nabla \cdot (\varepsilon_k (\sigma'_k)^k) - \frac{1}{\Delta V} \int_{A_k} \rho_k v_k (v_l - v_k) \cdot n_k dA_k
\]

\[
+ \frac{1}{\Delta V} \int_{A_k} \sigma'_k \cdot n_k dA_k + \varepsilon_k (\rho_k)^k X_k
\] (2.17)

The second term on the right hand side would represent momentum exchanges between all the phases and the \(k\)th phase due to phase change. Hence,
\[ - \frac{1}{\Delta V} \int_{A_k} \rho_k \mathbf{v}_k (\mathbf{v}_I - \mathbf{v}_k) \cdot \mathbf{n}_k dA_k = \sum_{j=1, j \neq k}^{\pi} \langle \dot{m}_{jk}^m \rangle (\mathbf{v}_k^I)^k \]  

(2.18)

The third term is also another term that results from averaging and represents the momentum exchange between phases and can be represented as a source term:

\[ \frac{1}{\Delta V} \int_{A_k} \sigma_k' \cdot \mathbf{n}_k dA_k = \sum_{j=1, j \neq k}^{\pi} \langle S_{jk} \rangle \]  

(2.19)

\( \langle S_{jk} \rangle \) is the interactive force that depends on drag (friction), pressure and cohesion between phases.

From Newton’s third law we know that

\[ \langle S_{jk} \rangle = - \langle S_{kj} \rangle \]  

(2.20)

And it can be modeled as

\[ \langle S_{jk} \rangle = K_{jk} (\langle \mathbf{v}_j \rangle^I - \langle \mathbf{v}_k \rangle^k) \]  

(2.21)

\( K_{jk} \) is the interphase momentum exchange coefficient.

We can drop the averaging symbols, \( \langle \quad \rangle \), from equation 2.17 and use the subscript \( s \) to denote the solid phase and no subscript to denote the fluid phase, we get the recognizable volume averaged equations.

\[ \frac{\partial}{\partial t} (\varepsilon \rho \mathbf{v}) + \nabla \cdot (\varepsilon \rho \mathbf{v} \mathbf{v}) = \nabla \cdot (\varepsilon \sigma) + \mathbf{S}_g - \varepsilon \rho \mathbf{g} \]  

(2.22)

Similarly, for the solid phase

\[ \frac{\partial}{\partial t} (\varepsilon_s \rho_s \mathbf{v}_s) + \nabla \cdot (\varepsilon_s \rho_s \mathbf{v}_s \mathbf{v}_s) = \nabla \cdot (\varepsilon_s \sigma_s) + \mathbf{S}_s - \varepsilon_s \rho_s \mathbf{g} \]  

(2.23)
2.2 Model A and B

Clearly, we have to find ways to close the above equations with respect to the source term. As Jackson\textsuperscript{11} has pointed out, the decomposition of the source term must correctly account for the buoyancy.

Model A:

\[
\frac{\partial}{\partial t}(\varepsilon \rho v) + \nabla \cdot (\varepsilon \rho v v) = -\varepsilon \nabla p + \nabla \cdot (\varepsilon \tau) + \beta_A (v_s - v) - \varepsilon \rho g \tag{2.24}
\]

\[
\frac{\partial}{\partial t} (\varepsilon_s \rho_s v_s) + \nabla \cdot (\varepsilon_s \rho_s v_s v_s) = -\varepsilon_s \nabla p + \nabla \cdot (\varepsilon_s \tau_s) + \beta_A (v - v_s) - \varepsilon_s \rho_s g \tag{2.25}
\]

And Model B:

\[
\frac{\partial}{\partial t}(\varepsilon \rho v) + \nabla \cdot (\varepsilon \rho v v) = -\varepsilon \nabla p + \nabla \cdot (\varepsilon \tau) + \beta_B (v_s - v) - \varepsilon \rho g \tag{2.26}
\]

\[
\frac{\partial}{\partial t} (\varepsilon_s \rho_s v_s) + \nabla \cdot (\varepsilon_s \rho_s v_s v_s) = \nabla \cdot (\varepsilon_s \tau_s) + \beta_B (v - v_s) - \varepsilon_s \rho_s g \tag{2.27}
\]

Where \( p \) is the fluid pressure field and \( v \) is the particle volume. On first examination, the difference between the two models is that in model A, the pressure field is shared by both phases while in model B, the pressure field is present only in the continuous phase. Both models are equivalent. This can be shown by considering that under the condition of steady flow where there is no acceleration in both phases the equations in the primary flow direction, \( y \), reduce to,

\[
0 = -\varepsilon \frac{\partial p}{\partial y} + \beta_A y (v_s - v) - \varepsilon \rho g \tag{2.28}
\]

\[
0 = -\varepsilon_s \frac{\partial p}{\partial y} + \beta_{A,y} (v - v_s) + \varepsilon_s \rho_s g \tag{2.29}
\]

If both equations are summed we get the so-called manometer rule:
\[- \frac{\partial p}{\partial y} = (\rho \varepsilon + \rho_s (1 - \varepsilon)) g \]  \hspace{1cm} (2.30)

The manometer rule mathematically relates the weight of the bed to the hydrostatic pressure drop. Solving for the pressure gradient in equation 2.28 and substituting into equation 2.30 we have

\[- \left( \frac{\beta_{A,y}}{\varepsilon} \right) (v_s - v) = (1 - \varepsilon) (\rho_s - \rho) g = - \frac{\Delta p}{\Delta y}_{\text{friction}} \]  \hspace{1cm} (2.31)

Hence, the principal contribution to static pressure is the drag experienced by the particles.

Similar treatment is applied to model B, neglecting acceleration we get, for both phases:

\[0 = - \frac{\partial p}{\partial y} + \beta_{B,y} (v_s - v) - \varepsilon \rho g \]  \hspace{1cm} (2.32)

\[0 = \beta_{B,y} (v - v_s) + \varepsilon \rho_s g \]  \hspace{1cm} (2.33)

The sum of equation 2.32 and 2.33 also gives the manometer rule hence proving the equivalence of models A and B. Solving for the pressure gradient and combining with equation 2.31 we obtain a relationship between \( \beta_A \) and \( \beta_B \) as:

\[\beta_{B,y} = \frac{\beta_{A,y} \rho_s}{\varepsilon (\rho_s - \rho)} \approx \frac{\beta_{A,y}}{\varepsilon} \]  \hspace{1cm} (2.34)

In the limit of the particle density being 3 or more orders of magnitude larger than the fluid density, the relationship between the 2 models is further simplified.

### 2.3 Particle dynamics

One problem in modelling the dispersed (particle) phase through a hydrodynamic model as in equation 2.25 is that the closures for the solid stresses have to be found using the Kinetic Theory of Granular Flow (KTGF) as presented by Gidaspow. Additional equations for a granular temperature are used to calculate the solid stresses. Alternatively, equations 2.25 for the solid can
be discarded and the particles tracked individually in a Lagrangian sense. Usually model A is
coupled with the particle tracking and the hydrodynamic equations for the solid phase discarded
in favor of a particle dynamics type equation where the net force on the particle drives the motion
according to Newton’s law of motion for a rigid body. The forces acting on each particle include
far-field pressure, particle fluid forces (not limited to drag, may include virtual mass, liquid-bridge
and Basset history forces), normal and tangential contact forces and body forces as in equation
2.35

\[ m_i \frac{d\mathbf{v}_i}{dt} = -\nu_i \nabla p + F_d + \sum_j (F_{cn,ij} + F_{ct,ij}) + m_i g \]  \hspace{1cm} (2.35)

Also, to fully account for the 6 degree of freedom motion of the particles, rotational component of
motion is computed,

\[ I_i \frac{d\mathbf{\omega}_i}{dt} = \sum_j (R_i \mathbf{n}_{ij} \times F_{ct,ij}) \]  \hspace{1cm} (2.36)

The particle position is updated kinematically as

\[ \frac{d\mathbf{x}_i}{dt} = \mathbf{v}_i \]  \hspace{1cm} (2.37)

Where \( F_{cn,ij} \) and \( F_{ct,ij} \) are normal and tangential forces on the particle \( i \), exerted by particle \( j \). \( I_i \) is
the moment of inertia, \( \mathbf{\omega}_i \) is the angular velocity, \( R_i \) is the distance of the center of point of the
particle to the point of contact. The contact forces are modelled using either a hard-sphere or a
soft-sphere model. The hard-sphere model is collision-driven and is typically more efficient
computationally than the soft-sphere model which requires resolution of the deformation process.
We describe the both contact models.
2.3.1 Hard-sphere model

The hard sphere models involves the binary collisions of particle pairs. Figure 2-2 gives a typical hard sphere model sequence as presented by Wu, Zhan, Li and Lam.\textsuperscript{14}

First, for any given particle, neighboring particles are scanned to detect all possible contacts using information from the particle velocities and positions. Collision time, $T_{m,n}$ for all contacts is found using the velocity and position of pairs of particles and the lowest $T_{mn}$ is chosen to advance the flow. Particles are advance using their velocities and the collision time to the new position. The process ends by using the impulse expected on collision to calculate the new particle velocities post collision. In order to illustrate the details of the calculation of the effect of collisions, consider figure 2-3
Where $\omega_1, \omega_2$ are the angular velocities, $r_1, r_2$ are radii, $m_1, m_2$ are masses of both particles, $n$ and $t$ are the unit normal and tangent of the collision coordinate system, $J$ is the impulse on collision and $G$ is the relative translational velocity between the particles. The relative velocity, $v_{12}$ at the contact point is given by:

$$v_{12} = v_1 - v_2 - (r_1 \omega_1 + r_2 \omega_2) \times n$$

(2.38)

$r_1, r_2$ are radii of the particles. The normal and tangential unit vectors that define the coordinate system are:

$$n = \frac{x_1 - x_2}{|x_1 - x_2|}$$

(2.39)

$$t = \frac{v_{12}^0 - (G_{12}^0 \cdot n)n}{|v_{12}^0 - (G_{12}^0 \cdot n)n|}$$

(2.40)

The subscript 0 denotes conditions before collision.

$$G_{12} = v_1 - v_2$$

(2.41)

The following equations are then used to calculate the post-collision velocities:

$$m_1(v_1 - v_{10}) = J$$

(2.42)

$$m_2(v_2 - v_{20}) = -J$$

(2.43)

$$\frac{l_1}{r_1}(\omega_1 - \omega_{10}) = J \times n$$

(2.44)

$$\frac{l_2}{r_2}(\omega_2 - \omega_{20}) = J \times n$$

(2.45)

$l_1, l_2$ are moments of inertia of the particles. Combining and noting that $B_1 = \frac{7}{2}(\frac{1}{m_1} + \frac{1}{m_2})$ and $B_2 = \frac{1}{m_1} + \frac{1}{m_2}$ we get an expression for the relative velocity before and after collisions:
\[ v_{12} - v_{12}^0 = B_1 J - (B_1 - B_2)(J \cdot n)n \] (2.46)

Using the appropriate material properties such as the normal and tangential restitution coefficients \((e_n, e_t)\) and the coefficient of friction, we can obtain expression to calculate the post collision relative velocity and the impulse:

\[ v_{12} \cdot n = -e_n(v_{12}^0 \cdot n) \] (2.47)

Thus

\[ J = -(1 + e_n) \frac{v_{12}^0 \cdot n}{B_2} \] (2.48)

If the coefficient of friction is less than the tangential component of the collision – i.e. \(\mu_f < \frac{(1+e_t)v_{12}^0 \cdot t}{J_n B_1}\) then gross sliding occurs and the sliding impulse is calculated as

\[ J_{t,sliding} = -\mu_f J_n \] (2.49)

If however \(\mu_f > \frac{(1+e_t)v_{12}^0 \cdot t}{J_n B_1}\), sticking occurs and we get

\[ J_{t, sticking} = -(1 + e_t) \frac{v_{12}^0 \cdot t}{B_1} \] (2.50)

2.3.2 Soft-sphere model

By contrast to the hard-sphere model, the soft-sphere model for particle-particle interactions is a time-driven strategy in which the particles are allowed to slightly overlap and the tangential and normal forces are calculated based on the extent of this overlap. Figure 2-4 gives an idealization of the contact force as a spring-dashpot system.
Because of the time-driven approach employed in calculating particle-particle interactions, the algorithm is much simpler than that for the hard-sphere collision algorithm. Wu, Ayeni, Berrouk and Nandakumar\textsuperscript{15} describe the linked-cell algorithm. It begins by dividing the entire computation domain into cells the same size as the particle (or the size of the largest particle in a polydisperse system). The 27 cells in the vicinity of the particle are then scanned for other particles and collision is detected if the centers of the particles in the surrounding search grid are less than 2 times the particle radius. A collision list of all particle contacts is built during each DPM time-step and the associated inter-particle forces are calculated using any of the available models. The forces are then integrated in time and the simulation is advanced.

The various approaches for calculating the contact forces in a soft sphere sense include viscoelastic models such as the Linear Spring-Dashpot-Slider model\textsuperscript{16} and the Hertz-Mindline model\textsuperscript{17} and elastic-plastic models like the Walton-Braun model\textsuperscript{18}.

2.3.2.1 Linear spring, dashpot and friction slider

In this model, the effective normal and tangential spring stiffness’s, $k_n$ and $k_t$ for a particle pair is simply taken as the arithmetic mean of their individual springs stiffness’s: $k_n =$
Likewise, \( k_t = 0.5(k_{t,a} + k_{t,b}) \). These expressions can be used without modification to calculate the contact forces in equation (contact force equation).

2.3.2.2 Non-linear Hertzian Model

It is expected that an increase in overlap of the colliding particles should result in an increase in area of contact. This leads to the belief that there should exist a non-linear expression for the spring stiffness and the contact force. As stated in the literature, the contact force in this model bears a non-linear relationship with the overlap between the two particles and a non-linear spring stiffness. The contact force in equation 2.35 is given as follows:

\[
F_{ab} = -(k_{ab,n} n_{ab} - \eta_{ab,n} v_{ab}) \delta_n^{p} \tag{2.51}
\]

The exponent, \( p \), is usually taken as 3/2. \( k_{ab,n} = \frac{E_a E_b r_{eff}}{E_a(1-\nu_a^2) + E_b(1-\nu_b^2)} \). Where the effective particle radius is \( r_{eff} = \frac{r_a r_b}{r_a + r_b} \). \( E_a, E_b, \nu_a \), and \( \nu_b \) are the Young’s modulus’s and Poisson ratios of the two particles of interest respectively. The damping constant is given as \( \eta_{ab} = \frac{3k_{ab,n}(1-e_{ab,n}^2)}{4|v_{ab}|} \).

2.3.2.3 Elastic-Plastic Model

Other than visco-elastic models, elastic-plastic models can also be invoked to model the particle-particle interactions while capturing the loss of energy due to collisions. As an example, the Walton plastic model has two components that encapsulate the loading and unloading history of the force-displacement relationship and the rate of change of the various components of the contact force. Loading is defined when the rate of change of displacement is negative (opposite the direction of the contact force) and unloading when the reverse is true. Hence for the normal force:

\[
F_n = \begin{cases} 
-k_1 \delta_n n_c, & \delta_n \geq 0 \\
-k_2 (\delta_n - \delta_{n0}) n_c, & \delta_n < 0 
\end{cases} \tag{2.52}
\]

And the tangential force:
\[
F_t = \begin{cases} 
F_t' + k_t^0 \left( 1 - \frac{F_t - F_t^*}{\mu F_n - F_t^*} \right)^{1/3} \Delta v_t^e, & \text{if } \dot{v}_t \text{ is in initial direction} \\
F_t' + k_t^0 \left( 1 - \frac{F_t - F_t^*}{\mu F_n + F_t} \right)^{1/3} \Delta v_t^e, & \text{if } \dot{v}_t \text{ is in opposite direction} 
\end{cases}
\]

Where \( F_t = |F_t|, F_t^* = 0 \) when time is 0 and set to \( F_t \) when \( \dot{v}_t \) reverses direction.

2.3.2.4 Contact Time

An issue of interest in soft sphere modeling of discrete particles is the time of contact and how it affects the choice of the time-step in the numerical implementation. The solution to equation (spring-dashpot-slider equation) if recast in 1-dimensional space is given in Van der Hoef, Ye, Van Sint Annaland, Andrews IV, Sundaresan and Kuipers

\[
\delta_n(t) = \frac{u_{ab,0}}{\Omega} \exp(-\Psi t) \sin(\Omega t) \tag{2.53}
\]

\[
\dot{\delta}_n(t) = \frac{u_{ab,0}}{\Omega} \exp(-\Psi t) \ast (-\sin(\Omega t) + \cos(\Omega t)) \tag{2.54}
\]

Where \( u_{ab,0} \) is the initial relative velocity and \( \Omega = \sqrt{\frac{k_n^2}{2m_{eff}}} ; \Psi = \sqrt{\frac{\Omega_0^2 - \Psi^2}{\Omega_0}} \) and \( \Omega_0 = \frac{k_n}{\sqrt{m_{eff}}} \). If the equation for the overlap is set to zero (\( \delta_n = 0 \)) the duration of contact, \( t_{contact} \) can be obtained.

\[
t_{contact} = \frac{\pi}{\Omega} \tag{2.55}
\]

It is important from a computational standpoint to properly choose the value of the DEM time-step at least half this value so that the calculation of the overlap would not be unphysically large. Key to this is our choice of the material properties \( k_n \) and \( k_t \). Van der Hoef, Ye, Van Sint Annaland, Andrews IV, Sundaresan and Kuipers mention that the values of \( k_n \) and \( k_t \) chosen could purely reflect a need to keep the particle overlap to a reasonable fraction of the particle radius rather than to ensure rigorous modeling of the inter-particle interactions.
The net torque acting on a particle j with radius \( r_a \) is given as:

\[
T = \sum_j r_a n_{ij} \times F_{ij,t} \quad (2.56)
\]

In order to justify the addition of the added mass force, density ratio must be low: \( \rho_p / \rho \ll 1 \). This was not the case for the suspensions studied and in order to improve computation efficiency, this effect was not included.

The benefit of using the soft-sphere model over the hard-sphere model is that multiple particle contacts can be accommodated in calculating the inter-particle forces as opposed to the binary collisions allowable for the hard-sphere model. One drawback is the computational inefficiency that may be introduced when we select a low DPM time-step. Usually the timestep for P-P interactions should be 1 order of magnitude less than the characteristic contact time. An estimation of this contact time based on the stiffness constant, \( k \), is:

\[
t_{contact} = \sqrt{k/m_{eff}} \quad (2.57)
\]

2.4 Discretization of the volume-averaged equations for a flow solver

The finite-volume method is used for the spatial discretization of the volume-averaged equations of motion. In order to model the DEM-CFD method the first instinct is to reorganize the volume averaged equations of motion to look like those of the single-phase equations of motion with a source term that can be easily plugged into a commercial CFD solver like fluent, i.e.:

\[
\frac{\partial \rho}{\partial t} + \nabla (\rho \mathbf{v}) = S_c \quad (2.58)
\]
And the momentum equation becomes:

\[
\frac{\partial}{\partial t}(\rho v) + \nabla \cdot (\rho \mathbf{vv}) = -\nabla p + \nabla \cdot (\mathbf{r}) + \rho \mathbf{g} + S_m
\]  

(2.59)

Where \( S_c = -\rho \left( \frac{\partial \varepsilon}{\partial t} + \mathbf{v} \cdot \nabla \varepsilon \right) \) while the momentum source term is \( S_m = S_c \mathbf{v} + \frac{1}{\varepsilon} (S_p + \mathbf{r} \cdot \nabla \varepsilon) \).

The source term resulting from interaction with the discrete phase is \( S_p = S + S_a \). The source term can thus be applied into the commercial CFD solvers like FLUENT, Star-CD, CFX and OpenFOAM where the source terms can be calculated implicitly with other flow variable like the velocity field and pressure field calculation. However because this implementation is not based on the integral form of the governing equations they cannot be relied upon to guarantee mass balance and the discretization should begin not from the differential form of the governing equations but from other integral momentum and mass balance \(^{21}\). If we consider a general property \( \psi \) and write the transport equation for two-phase flow we have

\[
\frac{\partial}{\partial t}(\varepsilon \rho \psi) + \nabla \cdot (\varepsilon \rho \mathbf{v} \psi) = \nabla \cdot (\varepsilon \Gamma \nabla \psi) + S_\psi
\]  

(2.60)

\( \Gamma \) is the diffusivity. If we integrate over a control volume \( \Delta V \) and reorganizing the equation to yield a new implementation of the source term

\[
\frac{(\rho \psi)^{n+1} - (\rho \psi)^n}{\Delta t} \Delta V + \sum_f \psi_f \Lambda_f = \sum_f D_f + S_\psi \Delta V
\]  

(2.61)

The source term, \( S_\psi \) is \( S_\psi = -\frac{1}{\Delta t} (\rho \psi)^n (1 - R_t) + \frac{1}{\Delta V} \sum_f (1 - R_f) (\Lambda_f \psi_f - D_f) + \frac{S_\psi}{\varepsilon_P} \). The indexes \( n+1 \) and \( n \) indicate the current and previous time levels respectively. The diffusive flux, \( D_f = \Gamma_f (\nabla \psi) \mathbf{r}_f \cdot \mathbf{A}_f \), the convective flux, \( \Lambda_f = \rho \mathbf{v}_f \cdot \mathbf{A}_f \), the “void fraction temporal ratio” and “void fraction spatial ratio” at cell face are defined \( R_t = \varepsilon_p^n / \varepsilon_p^{n+1} \) and \( R_f = \varepsilon_f^{n+1} / \varepsilon_p^{n+1} \). An accurate calculation of the void fraction gradient especially at the cell face is necessary to ensure mass
conservation. Even though the system of interest is a closed system where the calculation of the overall net flux is not critical to a meaningful result as with a fluidized bed, Wu, Nandakumar, Berrouk and Kruggel-Emden note that this solution strategy can help in enhancing solution convergence.

The discretized momentum equation in direction \( i \) is given in the following form:

\[
\bar{a}_P v_{i,P} = \sum_{nb} \bar{a}_{nb} v_{i,nb} + \varepsilon \sum_f p_f A_i + S_i \tag{2.62}
\]

\( \bar{a}_P \) contains the coefficient of the fluid velocity in the expression of the source term hence ensuring the implicit calculation of the momentum source. If the pressure field and face mass fluxes are known, the velocity field can be obtained. We can’t know the pressure field beforehand because it is coupled to the velocity field. The collocated grid algorithm of Rhie and Chow where both the pressure and velocity field values are stored at the cell center means an accurate method for calculating the face values should be used.

It is also noted that the method for calculation of the volume fraction uses a fully analytic method according to Wu, Zhan, Li, Lam and Berrouk. The analytic method would ensure smooth field of the volume fraction and enhance the calculation of the source terms calculations utilized in the continuous phase calculations Wu, Zhan, Li and Lam.

A first-order implicit scheme was used for temporal discretization.

The pressure-velocity coupling is handled in a segregated fashion by employing the SIMPLE algorithm. A pressure field is guessed and used to obtain a first estimate of the velocity field. This velocity field is used to constitute a system of equations for the domain from the continuity equation called the pressure correction equation. The pressure correction is then used
to obtain a more accurate estimation of the pressure and velocity field and pressure field. The Algebraic multi-grid method is applied to the pressure correction equation.

2.5 Source terms and numerical stability

The flow variables except the source terms are calculated implicitly. The source term is linearized and treated in a “semi-implicit” fashion.

\[ S^{n+1} = A^n \mathbf{v}^{n+1} + B^{n+1} \] (2.63)

\( A^n \) is given as \( A^n = -\sum_{k=1}^{NPC} V_{p,k} \beta^n / V \) and \( B^{n+1} = \sum_{k=1}^{NPC} V_{p,k} \beta^n \mathbf{v}^{n+1} / V \). \( B^n \) depends on \( \mathbf{v} \). Therefore, in order to linearize the source term, \( \beta \) is calculated at the previous time-step hence the semi-implicitness. It can be seen that the value of magnitude of \( A^n \) is always positive when added to the coefficient of \( u_{i,p} \) in the discretized equation. It therefore preserves convergence as it makes the system of equations for solving the velocity field more diagonally dominant and hence improving solution convergence 14.

In order to calculate the face centered value of the field variables, a second-order upwind differencing scheme is used.

\[ \varphi_f = \varphi_{r,upwind} + \nabla \varphi_{r,upwind} \cdot d\mathbf{r} \] (2.64)

The numerical stability of the source term calculation especially for strongly coupled systems with high volume fraction must include the use of an underrelaxation factor, \( \alpha \) which is between 0 and 1 24.

\[ S = S_{old} + (1 - \alpha)S_{new} \] (2.65)
The value of the under-relaxation does not affect the accuracy of the final converged solution; this is controlled by the specified tolerance, time-step and degree of coarseness of the spatial discretization.

2.6 Discretization of particle dynamic equations

The particle dynamic equations given in equation 2.35 are discretized in an implicit fashion according to equation 2.66 below

\[
\frac{m_p(v_p^n - v_p^{n+1})}{\Delta t} = -V_p(\nabla p)^{n+1} + \frac{V_p\rho^n_p}{1 - \varepsilon^{n+1}}(v^{n+1} - v^n_p)
\] (2.66)

In the equation, the contact forces have been omitted. The current velocity of the particle, \(v_p^{n+1}\), is replaced by an intermediate velocity, \(v_p^*\). The source term for the fluid coupling are calculated using this abridged form of the particle dynamic equation until convergence is achieved. After which, the entire particle fluid force is calculated as, \(F_{f-p}\)

\[
F_{f-p} = \frac{m_p(v_p^* - v_p^n)}{\Delta t}
\] (2.67)

Then finally this fluid-particle force is incorporated into the entire particle dynamic equation to update particle positions as follows:

\[
\frac{m_p(v_p^{n+1} - v_p^n)}{\Delta t_{DPM}} = F_{f-p} + \sum_j (F_{cn,pj} + F_{ct,pj}) + m_p g
\] (2.68)

Wu, Ayeni, Berrouk and Nandakumar\(^1\) point out a number of benefits of this strategy. It ensures the particle-fluid calculations are completely decoupled from the particle-particle calculations and thus allows robust code modulation for Eulerian as well as Lagrangian calculations. It also ensures that the exact magnitude of the particle-fluid force calculated for the fluid is the same as that used for the particle calculations despite the, sometimes, large difference
in time-scale for the fluid calculations and DPM calculations. This guarantees satisfaction of Newton’s third law of motion. Above all it ensures that there is implicit coupling between the CFD and DPM calculations since the source term is calculated iteratively.

2.7 Implementation of Source Terms In Fluent

Fluent is an industry standard software used primarily for solving fluid flow. It hosts options for solving the mass, momentum, energy and species transport equations. The multiphase flow models implemented in fluent include the two-fluid model, Volume of fluid model, discrete phase model and the mixture model. The in-built discrete phase model is compared to the DEM model used in this work. The discrete phase model explicitly tracks the dispersed phase and can handle high mass loading but not high volume fractions and high particle collisions.

Because the density ratio between the liquid and solid phase is $O(1)$, the momentum coupling has to be handled implicitly. Fluent allows for a straight-forward implementation of the momentum source term using a user-defined interface written in C. Fluent like many other flow solvers is not designed to handle the specifics of every flow problem and hence allows for the customization of boundary conditions, material properties and sources and sinks in the governing physical equations. Due to the tight coupling between the pressure and velocity terms in the SIMPLE algorithm, the pressure field must be calculated implicitly. The source terms must be linearized and coefficients absorbed into matrix of the coefficients of the cell centered velocities. The source terms must be related to the void fraction and the gradients of the void fractions on each cell especially for dense particulate flows. Fluent allows for the storage of additional cell properties like the void fraction as User-defined scalars and automatically calculates their gradients.
There are two time layers to be considered in the solution of any DPM-CFD problem: the fluid time-step, $\Delta t$ and the DPM time-step, $\Delta t_{DPM}$ which should be at least one order of magnitude smaller than the fluid time-step. The stiffness of the system of equations to be solved is by a first approximation $O\left(\frac{\Delta t}{\Delta t_{DPM}}\right)$. In order to preserve computational efficiency, this ratio must not be set too high but allowance should be made so that it is not too low as to result in unrealistic overlap between particles and unnatural values for the inter-particle forces. At the beginning of the iteration, the particles are assumed fixed in space and the volume fraction and its gradient are calculated. A bulk of the computational time is spent in the volume fraction calculation and hence it is calculated only once per fluid time-step. The particles are advanced in time using the rigid body equations and accounting for the drag and particle-particle interactions. The source terms are calculated based on the slip velocity of the particle relative to the fluid phase and the fluid phase momentum equation is solved by the flow solver. Selection of the time-step should be $O(1)$ less than the particle response time to accurately model the particle response to the fluid\textsuperscript{25}. The particle response time is given as: $\tau_p = \frac{\rho_p d_p^2}{18\mu}$. An advantage of the time-driven soft-sphere modeling strategy is that we do not need to wait till the end of the calculation of the fluid flow equations to calculate the particle interactions unlike the hard-sphere model. The particle equations can be solved alongside the fluid equation with the inter-particle forces integrated over time. This permits us to use the domain decomposition for parallel computation. The work flow (figure 2-5) for the coupled DPM-CFD procedure is generic for both dense particulate flow (where volume fraction and collision effects are modeled) and dilute flow ($\varphi \leq 0.1$) and reflects the implicit coupling of both phases.
2.8 Parallel computing considerations

The parallelization of CFD solvers often follows the domain decomposition approach by dividing the computational domain into any number of partitions of comparable computational cell count. The computational task for each of the subdomains arising from this parallelization is then farmed off to one logical computing unit. Usually, the computational grid within each subdomain does not change for the entire life of the simulation and traditional parallel approach perform well for such systems. However, for dynamic particulate systems where the distribution of particles is not homogenous throughout the computation domain, using a traditional domain decomposition approach may lead to load balance problems. Consequently, there arises a need to implement a parallelization procedure that takes into account the lack of uniformity in the distribution of the dispersed phase. One such method is the hybrid scheme implemented by Wu, Ayeni, Berrouk and Nandakumar which incorporates both spatially uniform domain decomposition using a message passing (MPI) paradigm and a multithreaded parallelism using a
shared memory (OpenMP) paradigm. The DPM-CFD coupling module implements a Single Input Multiple Data strategy where global property variables of the physical system are hosted on the host node and . Input output operations and global reduction operations of integrated properties are performed on node 0 while computations on unique subsets. Data storage and computational tasks are assigned to compute nodes if particles are hosted by the compute node.

The parallel scalability of the code is tested on the Queen Bee hpc cluster hosted by Louisiana Optical Network Initiative. It features a 50.7 TFlops peak performance 680 compute node cluster. Each node is fitted with the two intel Quad-core Xeon 64-bit processors at a core frequency of 2.33GHz. Parallel communication is achieved over a high latency 10Gb/sec infiniband interconnect network interface. The physical system used to test the parallel scalability consists of a fixed bed of 1,021,977 particles and 524,288 fluid computational cells. Fluid is introduced through a uniform inlet at the bottom of the bed against gravity at a rate below the minimum fluidization velocity. Figure 2-6 shows the comparison of the speed-up achieved with multi-threading and without multi-threading. A relatively faster speed up attained due to multithreading is obtained because of less time devoted to fewer communication activities under a shared memory architecture.

![Figure 2-6: Parallel Speedup for increasing number of cores](image)

28
Chapter 3 Behavior of Clusters of Particles in a Viscous Ambient Fluid

3.1 Introduction

When a phase is distributed in another but is not materially connected to it, the system is called dispersion. Dispersions of solid particles suspended in a fluid of lesser density tend to settle out of suspension because of the density difference that exists between the dispersed and the continuous phase in a process called sedimentation. Sedimentation is thus a multi-phase description that differs from multicomponent flow where the constituents are mixed on a microscopic scale.

Sedimentation is an important process employed in many industrial processes and is utilized in processes where the density and size distributions of suspended particles can be exploited for phase separation. Processes such as the clarification of sugar bagasse, water treatment or pre-treatment of metal ores all employ this principle.

Some large-scale natural occurrences that involve sedimentation include the flow of solid and liquid in volcanic eruptions, flow of sediment down a slope in lakes and the open water disposal of sediments and dredging of coastal waters. An understanding of the dynamics of particle dispersion in a liquid solid system can help improve placement of sand and reduce the number of times dredging activities have to be carried out. On a smaller scale, deposits of fat inside arteries and flow of blood corpuscles also fall under liquid-solid flows and involve sedimentation.

Other liquid solid systems that require some knowledge of sedimentation include industrial activities such as hydro-transport of particles like coal, or cuttings that result from drilling activities.
in the oil and gas industry. Also of interest is the transport of micro-sensors to fractures within rock formations that would report back information about the nature of the formation.\textsuperscript{29}

The density imbalance in a liquid-solid mixture ensures that the system continues to evolve until observable segregation takes place e.g. the fluid at the top of the vessel becomes clear and the suspension at the bottom becomes more concentrated. Even though the buoyancy and the drag on the individual particle act at the microscopic scale, they influence interesting large-scale dynamics of the system.

Sedimentation is naturally a “non-equilibrium” phenomenon. Unlike in fluidization where steady state can be described as the point at which the drag exerted on the particles by the inlet fluid stream balances the weight of the bed, thus allowing us to describe a minimum fluidization velocity, we cannot physically describe an equilibrium point in sedimentation except for theoretical investigations where a periodic boundary condition is used in the direction of gravity\textsuperscript{30} or the system is neutrally buoyant thus permitting the equilibrating effect of Brownian fluctuations. The focus of this part of the work would be on particle-liquid systems where the density ratio is substantially greater than one and on inhomogeneous sedimentation where the volume fraction of solids is confined to a finite volume within the clear continuous phase as idealized in figure 3-1.

The complete description of the inter-particle, hydrodynamic, thermal and external forces acting on a suspension of particles and their spatial distribution is known as the microstructure.\textsuperscript{31} The microstructure and the statistics of the suspension evolve with time to become increasingly disorderly. We may simplify the model by legitimately assuming that particles studied in all
simulations are large enough for Brownian effect to be neglected and that some form of continuum description of the fluid can be obtained based on the volume fraction of the phases.

Figure 3-1: Homogeneous (left) and inhomogeneous (right) dispersions

The concern in this work is with the fundamental problem of the sedimentation of a cloud of particles in an otherwise clear liquid. The terms cloud, blobs and suspension drops are taken to mean an initially spherical swarm of solid particles in a viscous fluid. As the cloud settles under the influence of gravity, a number of things could occur including particle leakage \(^1\) and pattern formation due to breakup \(^32\) depending on the flow conditions. Traditionally, the method of simulation has been to use a description that preserves the linearity of the governing equations for the fluid phase e.g. using Stokeslet simulations or Oseenlet simulations which are slight variation of the Stokeslet \(^1, 26, 33, 34\). By contrast, the model used in this work, the finite volume – lagrangian tracking approach deployed does not neglect the non-linear inertia term in the governing equation.

The aim of this work is to investigate the breakup features of a settling cloud and analyze the effects of inertia, initial volume fraction, nature, size and shape of the boundaries and material properties on the shape instabilities of the blob. Some of these effects have been studied in the context of homogenous sedimentation and at low Reynolds numbers. The significance of isolating
the behavior of a cloud is in the broader picture of analyzing the effect of cluster formation and persistence on the dynamics of homogenous sedimentation and multiphase systems in general where one phase is dispersed in another. Mixing and Segregation are issues that are also directly impacted by the behavior of particle blobs.

A summary of some of the various studies that have been performed regarding both homogeneous and inhomogeneous sedimentation are presented in section 3.2. The statistical tools for analyzing the evolution of particle clouds are introduced. Section 3.4 focuses on the validation of the simulations against data from experiments and theoretical formulations as presented in the literature and analysis of the results. We conclude chapter 3 in section 3.5.

3.2 Literature review

In contrast to gas-solid system where inter-particle collisions are frequent and the solid phase can be modeled as an ideal gas using the kinetic theory for granular flow \(^{12}\), the dynamics of liquid solid systems are dominated by long-range hydrodynamic interactions. If the particle diameter is >10\(\mu\)m, the effect of thermal fluctuations in the fluid phase can be neglected in deference to the hydrodynamic interactions \(^{35}\). Research into liquid solid systems is not new and the focus has ranged from instabilities in the structural patterns of settling swarms of particles to the influence of boundaries on the fluctuation of particle velocities around a mean value.

A number of methods have been employed to model liquid solid systems: Lattice-Boltzmann simulations \(^{36}\), Direct Numerical Simulations \(^{37}\), Two-fluid interpenetrating continua \(^{2}\), Stokesian dynamics \(^{1,26}\) and Spectral Methods with particle tracking \(^{32}\).

When the particles are uniformly distributed in a homogenous dispersion, the mean velocity would be less than the terminal settling velocity of a single particle. This phenomenon is
called hindered settling. Richardson and Zaki \(^{38}\) presented an expression that relates this hindered velocity of the suspension to the terminal settling velocity of the particle, \(u_0\) and some function of the volume fraction of solids in the suspension, \(\varphi\).

\[
u_s = f(\varphi) * u_0 \quad (3.1)
\]

They determined \(f(\varphi) = (1 - \varphi)^n\) where the exponent, \(n\) is close to 5 for small particle Reynolds numbers.

Batchelor \(^{39}\) focused on the theoretical determination of the mean value of the velocity of a sphere in a dilute suspension of identical spheres. In formulating the problem, the effect of inertia was neglected to preserve linearity of the system. If the probability distribution of a given configuration of particles is known we can determine the average of some quantity \(G\) associated with some position in the dispersion.

\[
\overline{G} = \frac{1}{N!} \int G(x, \mathcal{C}_N) P(\mathcal{C}_N) d\mathcal{C}_N \quad (3.2)
\]

\(\mathcal{C}_N\) is the configuration of a set of \(N\) identical particles and \(P(\mathcal{C}_N)\) is the probability density of the configuration. The key result of the work was to determine the correction to the average settling velocity. This value was found to depend on the size, shape, particle density and concentration of the suspension and proposed a correction to the settling velocity to be \(O(\varphi)\) in contrast to the \(O(\varphi^{1/3})\) dependence. Accordingly,

\[
f(\varphi) = 1 - 6.55\varphi + O(\varphi^2) \quad (3.3)
\]

The second term on the right hand side of equation 3.3 is due to the backflow of displaced fluid as the particles settle. There are difficulties in finding analytical solutions to the setting of a
dispersion of particles: The slow decay of the velocity disturbance produced in a fluid by a settling sphere goes asymptotically as $1/r$ where $r$ is the radius of the sphere; the random arrangement of particles in dispersion also makes calculations cumbersome. We can however overcome the difficulties of a rigorous analytical solution for sedimentation by employing an Eulerian-Lagrangian description of the flow. If the dispersion is described as a regular array of spheres (cubic, rhomboid etc.), the fractional reduction in fall speed is proportional to $\varphi^{-1/3}$ with a constant of proportionality that depends on the arrangement used. Batchelor $^{39}$ used a statistical-analytical approach to take into account the randomness of the configuration of particles in the dispersion.

He also pointed out that the difference between homogenous and inhomogeneous sedimentation is not in the presence or absence of rigid boundaries in the vicinity of the particles but the spatial variation of the statistical properties of the dispersion.

As opposed to hindered settling, a phenomenon which we could term “enhanced” settling occurs when a cluster of particles assumes a single identity thus causing the particles to settle many times faster than their individual terminal speed. Nitsche and Batchelor $^1$ and Favier, Abbaspour-Fard and Kremmer $^{40}$ presented an expression validated by the experiments of Kohring, Melin, Puhl, Tillemans and Vermöhlen $^{41}$ from theoretical analysis that is valid at low Reynolds number which shows the enhanced settling of a cluster of particles where the cloud velocity is $u_c$, the number of particles in the cloud is $N$ and the ratio of the particle radius to cloud radius is $\varepsilon$:

$$\frac{u_c}{u_0} = \frac{6}{5}N\varepsilon + 1 \tag{3.4}$$

A consequence of low Reynolds number is the slow particle leakage from the rear of a cloud. Nitsche and Batchelor $^1$ investigated the breakup of a falling drop of particles within this
limit. Multiple hydrodynamic interactions among particles cause random crossings of the imagined boundary of the blob – the loss of particles in the tail is a purely hydrodynamic effect. The Knudsen numbers are relatively high and thus no Brownian motion is involved in this random motion. The loss of particles in the tail of the blob is one mechanism in the smoothening out of the bulges that may have been present in the initial stages of sedimentation and may be an explanation why the breakup mechanism is not similar to that observed at higher Reynolds numbers where secondary droplets develop from these bulges \(^3\). The goal of their work was to observe the time evolution of a spherical blob and quantify the rate of leakage from the finite dispersion. They noted that the blob could fall in a manner resembling circulating halo of particles but without change to its compound spherical structure at low Reynolds numbers. A flux of particles across the interface of the cloud can be inferred from the leakage of particles as opposed to using a particle diffusivity of the conventional kind which would involve having an expression for the irregular surface of the blob. This can be modeled using Newton’s law of motion to calculate the acceleration of the particles while the hydrodynamic forces on a single particle are calculated from the torque-free solution to the Stokes equation for \(N\)-1 number of spheres. Clusters of particles can be regarded as an effective continuum with a density higher than the surrounding fluid. The difficulty in using the Stokeslet approach as noted by Nitsche and Batchelor \(^1\) lies in the unrealistically large ambient fluid velocity that could be calculated when two particle centers overlap. One method of solving this problem is to impose an artificial short-range repulsive force on each particle to keep them apart. This arbitrary force may be unnecessary and may modify the flow-field in an undesirable way \(^4\). Despite this relatively simple approach, the basic toroidal feature of cloud sedimentation can be reproduced. The rate of particle leakage is directly proportional to the single-particle terminal settling speed and inversely to the mean particle spacing to the fourth, \(d^4\), over a wide
range of initial particle numbers. \(-dN/dt = const \star u_0 R^2 a/d^4\) where \(R\) is the blob radius. This result is expected because the leakage rate should scale as the magnitude of the fluctuations, \(O(u_0)\), and be related to the area available for transfer of excess mass, \(O(R^2)\). Their simulations went up to a particle number of just 320 particles.

In a more recent paper, Pignatel, Nicolas and Guazzelli \(^{26}\) investigate the dynamics at small but finite Reynolds number. In order to properly characterize the flow regime of the cloud, they define a non-dimensional parameter which they call the “inertial length”, \(l^*\) which quantifies the ratio of viscous to inertia forces. \(l^* = (a/R)/Re_p - a\) and \(R\) are the particle and cloud radiiuses respectively. The particle Reynolds number is defined as \(Re_p = \rho U_0 a/\mu\) where the terminal velocity of a single isolated particle is \(U_0 = 2(\rho_p - \rho)a^2 g/9\mu\), \(g\) is acceleration due gravity and \(\mu\) is the liquid dynamic viscosity. On the basis of the inertial length, there are thus three identifiable flow regimes – the Stokes cloud regime where both \(Re_c\) and \(Re_p\) are <<1 (\(Re_c\) is Reynolds number of the cloud, \(Re_c = \rho v_c R / \mu\), where \(v_c = 6/5 U_0 (N_p \epsilon + 1), \epsilon = a/R\)); the macro-scale inertial regime where \(Re_c\) is no longer infinitesimal; micro-scale inertia regime (where both \(Re_p\) and \(Re_c\) are not small). In the Stokes regime, pure hydrodynamic interactions are sufficient to model the dynamics of the physical system. The particles can be treated as point forces and only far-field interactions are accounted for. The inertial length is highest in this regime. As we reduce the inertial length, we enter into the macro-scale inertia regime. The third and final regime, the micro-scale inertia regime deals with systems where both \(Re_c\) and \(Re_p\) are not negligible. Their studies focused on the last two regimes. By keeping the Stokes number \((St = 2/9 (\rho_p/\rho) \epsilon^2 Re_c)\) roughly the same in the number of parameters to be studied can be reduced to \(Re_c, N\) and \(l^*\).
Pignatel, Nicolas and Guazzelli 26 used a method of simulation called the Oseenlet simulations, which is a modification of the Stokeslet but contains an additional term to the steady state, reversible solution to flow around a sphere to model non-negligible inertia at long distances. Due to Oseen’s approximation, the Oseenlet remains linear but upstream and downstream symmetry is lost. The linearity permits a summation of the hydrodynamic disturbance to the flow field from multiple momentum sources. The dynamics of cloud settling using this method were found to be in agreement with those in other studies. As the cloud descends circulation within the cloud structure, expansion and eventual breakup of the cloud occur. This series of events is consistent under most flow conditions with only slight variations for each flow regime. They observe no particle leakage when the inertial length is small but as the inertial length is increased (corresponding to a reduction in the associated Reynolds numbers), particle leakage becomes a more quantifiable phenomenon. One highlight of their conclusions is that the mechanism for torus formation depends on the flow regime. At low $Re_c$, particle depletion along the vertical axis of the cloud causes the formation of torus while in the former, inflow of fluid at the rear of the cloud is
responsible. The difference between these 2 mechanisms is also what accounts for the absence of particle leakage at high Reynolds numbers as particles that would otherwise be lost in the wake of the descending cloud are conveyed back into the cloud by the recovering fluid. In addition, the breakup observed in a non-inertial regime is different from that in a high inertia regime. The cloud flattens as it descends, reaches a critical aspect ratio and loses its symmetry without evolving first into an open torus in the former while in the latter (this validates earlier experiments and simulations of Machu, Meile, Nitsche and Schaflinger 34), the fluid streamlines can pass through the center of the cloud creating an open torus well before the amplification of bulges on the torus and breakup.

Figure 3-3: Open torus showing fluid streamlines passing through the center. Only particles in the meridian plane are shown for clarity

They define an aspect ratio as the diameter of the cloud in the horizontal direction to the diameter in the vertical direction. The average settling velocity, growth of the aspect ratio of the particle cloud and break-up time at low Reynolds number regimes matches the experimental results presented but strong deviation is seen when the same comparisons are made at higher Reynolds number and higher volume fractions. This may be due to the nature of the modeling approach used.
which does not account for the effect of a finite particle volume and a possibility of increased frequency of collisions.

The role of particle-particle interactions in shape evolution of a cloud of particles was explored by Metzger and Butler \(^43\) who considered the influence of periodic shear flow on a neutrally buoyant cloud of particles that were close to the packing limit for mono-size hard spheres. The question they wanted to answer was whether the cloud of particles deformed through shear strain on the host fluid regains its original configuration upon reversal of the flow. In order to completely eliminate the effects of inertia, the fluid used was highly viscous. Advection therefore plays no part in the evolution of the cloud and the sole cause of departure from the initial shape of the cloud is inter-particle effects. By setting up their experiments they also wanted to clarify the significance of non-hydrodynamic interactions in modeling rheology of suspensions. Two factors govern the irreversibility or otherwise of the system: If the strain amplitude is above a critical value, the flow is irreversible; also, a close packing of the cloud at the start of the operation would mean that there has to be a dilation of the particle cloud as two adjacent layers of particles slide past each other. Reversibility seemed to be a feature of configurations that had sufficiently diluted or those with low enough volume fractions. The process produced interesting “galaxy” like shapes indicating that the core of particles moved as one entity while particles on the periphery are dispersed. They conclude that the reversibility of the time evolution of a cloud under imposed shear occurs below certain threshold concentrations constrained by the shear rate of the characteristic background flow points to the strong relationship between irreversibility and particle-particle collisions. They point out that long-range hydrodynamic interactions are not the only sources of chaos in particulate systems.
Mylyk, Meile, Brenn and Ekiel-Jezewska \cite{Mylyk2015} studied cloud destabilization in the presence of a hard vertical wall by performing experiments and stokes simulations. They found that the evolution of the cloud is fundamentally the same in an unbounded fluid but leakage is faster and the onset of destabilization is quicker. Most of their blobs broke up into 2 secondary blobs with a few into 3 blobs. The destabilization time and length were measured qualitatively as the time and distance when the open torus or flattened blob begins to bend. Their most important result was to find a linear correlation between the two quantities and the distance between the cloud centroid and the wall for both experiments and simulations. The experiments showed a slightly more cohesive behavior than their point particle simulations and this can be attributed to the liquid bridging that exist in liquid solid systems.

Regardless of the initial shape of the cloud, at low to moderate $Re_c$, the torus is the only intermediate shape before the cloud disintegrates. Streamlines of fluids do not immediately pass through the center of the torus after its formation and due to the formation of a “stream envelope” that encloses the streamlines within the cloud structure even when only a low density of particles is present in the hole of the torus. After some time has elapsed, the fluid streamlines pass through the center of the torus to form an “open torus”. This open torus is what is prone to disintegration. An explanation of the leakage of particles different from that presented by Nitsche and Batchelor \cite{Nitsche1975} is given. To explain the leakage of particles, they define a stream envelope as the imaginary surface separating the outer bypassing streamlines and the inner toroidal circulations within the cloud substructure. This is shown in figure 3-4. The envelope of closed streamlines extends partly outside the drop to permit recirculating particles in the core of the cloud to entrain the bypassing streamlines and be swept to the rear of the cloud and subsequently lost. An alternate and related explanation for the distortion of the flow path of the ambient fluid around the cluster of particles
is the high pressure region that develops at the leading front of the particle cluster. At the trailing front of there is an accompanying low pressure region that result from the pressure recovery of the flow-field in the ambient fluid.

Using a spectral method for the fluid phase while tracking particles in a lagrangian framework, Bosse, Kleiser, Hartel and Meiburg\textsuperscript{32} simulated the behavior of a settling cloud under a range of $Re_c$ from 0 to 100. In all simulations they use the standard drag coefficient for the description of the drag on each particle and the buoyancy force as the driving force of motion. Their Navier-Stokes equation was modified by a feedback source term into the fluid phase for the motion of particles with the source term applied at the particle centers. Other parameters explored by their simulations include the stokes number of a single particle based on its terminal settling speed, the Froude number on the scale of the cloud radius, $Fr$, and the ratio between the density of the solid and continuous phase, $\rho_p/\rho$ and the initial volume fraction of the blob, $\varphi$. The cloud Reynolds number places a more stringent constraint on the extent to which inertial forces dominate.
the system than does the particle Reynolds number and fixing this value as low to moderate ensured they remained within a viscous dominated regime. Their simulations produced several interesting patterns for the shape evolution of the blob. For reasonably low \( Re_c \), the blob retains its roughly spherical integrity and shows streamlines that enclose a vertical substructure within the blob. As they increased \( Re_c \), the blob shows increasing tendency to disintegrate into 2 or more blobs which themselves disintegrate in a cascade of secondary drops. Their study showed the underlying transitional nature of the sedimentation of a particle blob. There was also an observed increase in the number of secondary drops with \( Re_c \). They also exposed the role that the initial particle distribution plays in the ensuing instability. As long as perturbations to the initial spherical shape of the cloud are of the order of the mean particle spacing, different patterns can be triggered. Grid resolution was also mentioned as a possible mechanism for the number of secondary clouds produced.

Metzger, Nicolas and Guazzelli \(^{33}\) report that at low Re, if the velocity of settling is normalized by Stokes settling velocity, the velocity bears linear relationship with \( N^*/R^* \) where the normalized Number of particles is \( N^* = N/N_0 \) and normalized cloud radius is \( R^* = R/R_0 \). The rate of departure from the Hadamard Rybczynski streamlines was also studied and was found to scale as \( N_0^{-1/3} \). They also observed different shape evolution for oblate and prolate clouds where oblate clouds possess a tendency to show instabilities by transitioning through tori while prolate clouds tend to leak particles more readily. The prolate shaped cloud recovers the spherical shape and then evolves into a torus at longer times. Finally, a criterion for destabilization is proposed for the class of clouds they studied based on a critical aspect ratio. The aspect ratio, \( \gamma = \frac{\sqrt{\sum_{i=1}^{N} f_i (x_i - \bar{x})^2}}{\sqrt{\sum_{i=1}^{N} g_i (y_i - \bar{y})^2}} \) (point \((\bar{x}, \bar{y})\) is the center of the cloud and point \((x_i, y_i)\) is the location of particle \(i\).
while $f_i$ and $g_i$ are discrete probability distribution functions for particles in both the $x$ and $y$ directions). They found that when the aspect ratio reaches a critical value ($\gamma \geq \gamma_c = 1.64$), and for particle number between 1000 and 3000, the cloud simulations predict destabilization.

Swan and Brady\textsuperscript{45} showed that the nature of the boundary at the top wall affects the flow of particles. If the suspension is entirely closed, the rate of sedimentation drops as a result of the significant backflow that is generated by the fluid as the suspension settles. In the case of a channel that is left open such that fluid may flow freely into and out of the flow domain, the suspension settles faster than when the fluid is confined such that there is no net flow into the system.

Abade and Cunha\textsuperscript{46} were interested in the effect of polydispersity on the aggregated behavior of settling clouds and velocity fluctuations. Their method of simulation was using point particle stokeslets. They find that the lifetime of a blob with significant polydispersity is less than that of a comparative mono-disperse blob. In order to get an expression for the rate of particle leakage, they treat it as a continuum phenomenon by relating the flux of particles across the imaginary surface of the blob to the fluctuation of particle velocity around a mean which is the source of particles randomly crossing the imagined surface of the blob. Their result was an exponential relation between the rate of particle leakage and the number of particles left in the blob while it remains spherical as $-dN/dt \sim 3/4 N^{2/3} \epsilon^2$.

Davis and Acrivos\textsuperscript{47} studied the enhanced settling of particles due to inclined vessels. An increase in the cross-sectional area available to the upward flowing fluid when particles form layers of sediment on the wall leads to an increase in the sedimentation rate. They mention that the settling velocity can be predicted from the thickness of the sediment layer, a sedimentation Grashof
number and a Reynolds number provided the flow is laminar and there are no instabilities in the form of waves in the flow.

Table 3-1: Summary of research in particle cloud settling

<table>
<thead>
<tr>
<th>Ref</th>
<th>Experiment or Simulations</th>
<th>Method of Solution</th>
<th>Flow Regime</th>
<th>Phenomena Observed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nitsche and Batchelor 1</td>
<td>E &amp; S</td>
<td>Stokeslet</td>
<td>Stokes</td>
<td>Particle leakage</td>
</tr>
<tr>
<td>Pignatel, Nicolas and Guazzelli 26</td>
<td>S</td>
<td>Oseenlet</td>
<td>Micro and macro scale inertia</td>
<td>Leakage, breakup</td>
</tr>
<tr>
<td>Bosse, Kleiser, Hartel and Meiburg 32</td>
<td>S</td>
<td>Particle-tracking/spectral method</td>
<td>Stokes – macro scale inertia</td>
<td>Leakage, Coalescence</td>
</tr>
<tr>
<td>Metzger, Nicolas and Guazzelli 33</td>
<td>E &amp; S</td>
<td>Stokeslets</td>
<td>Stokes</td>
<td>Particle leakage</td>
</tr>
<tr>
<td>Kohring, Melin, Puhl, Tillmanns and Vermöhlen 31</td>
<td>E</td>
<td>Experiments</td>
<td>Stokes</td>
<td></td>
</tr>
<tr>
<td>44</td>
<td>E &amp; S</td>
<td>Oseenlet interactions</td>
<td>Macro-scale inertia</td>
<td>Break-up</td>
</tr>
</tbody>
</table>

3.2.1 Phases of cloud settling

Despite the smaller degree of mixing compared to turbulent thermals, three distinct phases that resemble those of the descent of a thermal can be observed at moderate Reynolds number – a short period just after the release of the cloud that we would call the acceleration period in the manner of Rahimipour and Wilkinson 27 where the motion of the cloud induced by gravity responds to the stationary background fluid through the drag this phase may be short depending on the $Re_c$ of the particle cloud and is characterized by very little expansion of the cloud; A self-preserving phase where the general structure of the cloud remains axisymmetric either as an open or closed torus with internally circulating vortices within the cloud sub-structure with accompanying lateral expansion of the cloud; and finally a transition phase where the cloud losses its axisymmetric geometry and breaks up into any number of secondary clouds with subsequent dispersion into the host fluid.
3.2.2 Velocity fluctuation

Of interest to researchers are the velocity fluctuations that arise in sedimenting systems. These fluctuations are one of many observable quantities in studying the nature of hydrodynamic multi-body interactions in liquid solid systems. A large body of literature is also devoted to the interplay between the magnitude of velocity fluctuations and the system size. Caflisch and Luke \(^{48}\) summed the hydrodynamic interactions of particles in a suspension and found that for a suspension with uniform concentration throughout the system domain, the fluctuating velocity of a test particle diverges indefinitely as we increase system size. This is at odds with the experiments of Nicolai, Herzhaft, Hinch, Oger and Guazzelli \(^{49}\) who found a saturation of the amplitude of velocity variance at system sizes greater than \(20\alpha\varphi^{-1/2}\). One suggestion to bridge the theory and experiment has been to try to identify methods by which the slowly-decaying \(O(1/r)\) interactions are made to decay more rapidly. These so-called “screening” mechanisms have been the subject of research. Koch and Shaqfeh \(^{50}\) have suggested that these screening mechanisms can be modeled in the same fashion as the screening of electrostatic charges in an ionic liquid such that the neighborhood of a test particle is neutrally buoyant to the macro-scale suspension density. There have been attempts to explain the saturation of velocity fluctuations and the search for physical screening mechanisms that could make this occur. Brenner \(^{51}\) put forward a mechanism by which hydrodynamic screening can be achieved by keeping the probability distribution of particles random and making \(u\) decay faster than \(r^{-1}\). He also makes the argument that the lifetime of particle clusters that appear in the system is important in determining the magnitude of the velocity fluctuations. The blobs in his simulations display certain features including stretching at initial times and swirling with the particles moving back and forth across the smallest dimension of the cell despite the low Reynolds number considered. Three-dimensional fluctuations were predicted.
despite the thin gap in one dimension of the cell. There was a dependence of the magnitude of fluctuations on the gap width. Particles near the wall displayed much smaller fluctuations than particles in the core of the blob.

Segre, Herbolzheimer and Chaikin\textsuperscript{52} found that the velocity fluctuations will depend on the system size if the system size is less than the correlation length, $\xi$. The horizontal and vertical correlation lengths are defined as the lengths over which vertical and horizontal velocities are correlated respectively. They found the dependence of horizontal Correlation length on volume fraction to be $\xi_\perp = 27a\varphi^{-1/3}$ and the vertical correlation length to be $\xi_\parallel = 11a\varphi^{-1/3}$. These quantities are related to the swirl size in the suspension. They also found the amplitude of the vertical velocity fluctuations to be twice that of the horizontal velocity fluctuations.

Guazzelli and Hinch\textsuperscript{53} posited that long-range interactions between particles are observed at low Reynolds number cause disturbances in flow field of a test sphere of radius $a$ and this and with a magnitude of $O(u_0a/r)$. If the influence of other particles in the spherical region of radius $R_c$ around a test particle is calculated summing the effects of their disturbances, the change in sedimentation velocity of the particle will be $O\left(\int \frac{u_0a}{r} ndV\right) = O \left(u_0\varphi \left(\frac{R}{a}\right)^2\right)$ where $n$ is the number density of particles and $V$ is the system volume. Settling velocity should therefore depend not only on the size but the shape of the container.

Kuusela\textsuperscript{30} studied the “steady state” characteristics of homogenous sedimentation. He was concerned with the “loss of memory” – a phrase coined to reflect the apparent chaotic nature of multi-body the particle fluid system – by tracking the velocity auto-correlation function as a function of time. By analyzing the integral of the velocity auto-correlation function over long time-scales, they were able to obtain values for horizontal and vertical self-diffusion. The latter were
found to be higher. They found the velocity fluctuations to be sensitive to the size of the container and find that the spatial correlation length decreases with an increase in the volume fraction. Sangani and Acrivos calculated analytically the drag force when a fluid flows through a periodic or regular array of particles and find a linear dependence on $\varphi^{1/3}$.

Rubinstein and Torquato looked at the slow flow of a viscous fluid through a random array of particles by recasting Darcy’s formula in an ensemble-averaged form and finding the upper and lower bounds for the permeability.

It is known that the correction to the Hadamard-Rybczinsky equation for the settling velocity of a suspension drop is $O(\varphi^{1/3})$ for an ordered suspension. However, a rigorous theoretical analysis for the Stokes settling velocity of a drop for a dilute suspension with no regular configuration is not straightforward.

3.2.3 Particle clouds and immiscible liquid drops and their similarities

Machu, Meile, Nitsche and Schaflinger explore the similarities between liquid drops and particle clouds in both experiments and simulations and clarify that suspension drops have to contain a sufficient number of particles before they can approximate the behavior of liquid drops. Their simulation was done in the manner of Nitsche and Batchelor where gravity is the sole generator of flow field and the particles are modeled as stokeslets. They also point out the problem of the unrealistic velocity field due to the singularity in the stokeslet calculation resulting from the overlap of 2 or more particles. The nature of the stokeslet approach is such that because the point-force solution goes as $r^{-1}$, a singularity is generated as the centers of 2 particles approach. Unlike their predecessors, they do not employ any modification to the stokeslet to prevent this overlap but
still end up with a reasonable flow field. Among some of the conclusions reached in their study was that the particle number influences the evolution into a torus.

3.3 Computational setup

3.3.1 Two-way coupling

In multiphase systems we need to model the interaction between all the phases. The exchange of momentum is of primary concern here but other types of interactions including the exchange of mass, energy might be important in other systems.

The type of coupling to be considered for the particle and fluid motion depends on the flow regime. The Stokes response time, $\tau_p$, is one parameter used to determine what flow regime we are in and it quantifies the response of the particle to the continuous phase flow field.

$$\tau_p = \frac{2\rho_p a^2}{9\mu}$$

3.5

The ratio of the fluid dynamic response time of the particle to the characteristic time scale of the flow is called the Stokes number and governs the nature of particle fluid coupling. In the case of a settling blob of particles the time scale of the flow is generally taken as $R/u_c^{1.32, 34}$. $R$ is the initial radius of the blob and $u_c$ is a velocity of the order of the cloud settling speed and is typically $\left(\frac{6}{5} N\epsilon + 1\right) u_0$ for low Reynolds numbers. The Stokes number is therefore $St = \tau_p \frac{u_c}{R} = \frac{2\rho_p}{9\rho} e^2 Re_c$. If $St$ is high, it means that the particle inertia is too great to be affected significantly by the fluid stream. If $St$ is low, it means the response of the particle to changes in the continuous flow equation is instantaneous therefore supporting a one-way coupling provided the volume fraction is low.
3.3.2 Initial and boundary conditions

Except where otherwise stated, the initial particle distribution is in a regular lattice with the inter-particle separation defined as \( (V_p/\varphi)^{1/3} \) where \( V_p \) is the volume of the particle. The boundary conditions used except otherwise noted is the impenetrable wall BC.

The physical model consists of mono-disperse micron sized particles, the continuous phase is an incompressible Newtonian fluid.

3.4 Results and discussion

3.4.1 Validation

The descent of the cloud was validated both qualitatively and quantitatively. The cloud displayed the evolution and transition that is known to occur at low and moderate numbers. At low Reynolds numbers cloud deformation is not pronounced but cloud evolution is primarily due to the leakage of particles from the rear of the cloud. At higher Reynolds number, the evolution of the cloud is first into an axisymmetric torus and subsequently the breakup of the cloud into any number of secondary blobs depending on the discretization (number of particles in each realization of the cloud) and the flow conditions. We shall present some qualitative results in the subsections that follow. We first proceed to reproduce the volume fraction dependence at low volume fractions and low \( Re_c \), particle leakage at low \( Re_c \) and torus formation and breakup at moderate \( Re_c \).

3.4.1.1 Volume Fraction Effect and Enhanced Settling

One typical characteristic of sedimentation is that the settling speed of particles is altered as a result of long (hydrodynamic) and short range (contact) forces from that of the isolated particle. In the case of inhomogeneous settling, the particles’ decent speed is enhanced as the cloud takes on a collective identity. The enhancement factor of the particle velocity is \( O(\varphi e^{-2}) \) and is
therefore directly proportional to the number of particles in the discretization and the inter-particle spacing taking into account the particle size. The fall speed is dependent on the volume fraction of the cloud of particles, the density ratio $\rho_p/\rho$ and viscosity of the host fluid. In the region of low volume fraction and low inertia, the settling speed has been determined through asymptotic analysis $^1$ and analytical solutions $^{42}$ and experiments $^{57}$ to be:

$$v^* = \frac{v_c}{u_0} = KN\epsilon + c = K\varphi\epsilon^{-2} + c \quad 3.6$$

Where $K = 6/5$ and $c = 1$. It is expected that as the volume fraction and $N$ go to zero (isolated particle) the velocity approaches the terminal speed and as the volume fraction and discretization increase, the collective identity of the blob becomes more important than the behavior of each individual particle. In order to verify the code, simulations were run at $Re_c < 0.01$; $Re_p \approx 0.000 \, 075$ and $St = 0.000 \, 157$. Other conditions of the simulations were $\rho_p/\rho = 2.1$. The volume fraction of the simulations being $\leq 0.1$ permitted us to use the DPM simulations without the inter-particle collision forces. At low volume fractions we can model the drag on each individual particle using the spherical drag law where the volume fraction of the dispersed phase does not contribute to the interphase momentum exchange parameter $^{17}$. We see from figure 3-5, B that the velocity of clusters of particles at different volume fractions increases to an asymptotic steady state velocity. The velocity of the particle cloud, $v_c$ is normalized by the terminal settling velocity $u_0$ to give a non-dimensional settling speed $v^*$. This normalized velocity is plotted against $N\epsilon$ related to the volume fraction as in figure 3.5, A. The value of the constant, $K$, in equation 3.5 is closely matched in the simulations.
Table 3-2: Comparison of $N\epsilon$ dependence of settling speed in theory and simulations

<table>
<thead>
<tr>
<th></th>
<th>Theory</th>
<th>Simulation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K$</td>
<td>1.2</td>
<td>1.17</td>
</tr>
</tbody>
</table>

Figure 3-5: (A) Steady-state settling velocity vs $N_p \epsilon$; (B) Settling Velocity dependence on volume fraction

The fluctuating velocity, $v'$ of each particle in a suspension which is the velocity around the mean settling speed was found to also be directly related to the volume fraction of the cloud. It is known that for homogenous suspensions that the amplitude of the fluctuations goes as the characteristic particle spacing, $\varphi^{1/3}$. We document the velocity fluctuations for a range of volume fractions on a logarithmic plot in figure 3-6. The gradient of the line is found to be $0.3304$ with an $R^2$ value of $0.9989$ which confirms that the vertical velocity fluctuations are directly proportional to $\varphi^{1/3}$. The amplitude of the steady state horizontal velocity fluctuations is also dependent on the volume fraction in a similar fashion with a gradient of $0.3432$ and an $R^2$ value of $0.9913$.

Figure 3-6: (A) Vertical velocity fluctuations with volume fraction dependence (B) Horizontal velocity fluctuations with volume fraction dependence
The fluctuating velocity is scaled by the terminal settling velocity of a particle in the fluid. We can relate $v'_{y\infty}$ to $\varphi$ by the following relation $v'_{i\infty} = k_i \varphi^{1/3}$. The degree of anisotropy in the x and y axes can be compared by comparing the ratio of the pre-exponential. $k_y$ (=11.151) is found to be almost 3 times the value of $k_x$ (=4.0707) indicating strong anisotropy even for a geometrically symmetric entity like a spherical blob. There was no need to compare the fluctuations in the z-direction because a domain with a square cross-section was used and it will essentially be the same as the amplitude of the fluctuation in x-direction.

3.4.1.2 High volume fraction simulations

Attempt has been made in literature to match Oseenlet simulations to experiments at conditions where the volume fraction of solids is close to 0.5\(^{26}\). The fundamental problem in using this approach is that at high volume fractions, the inter-particle effects can no-longer be ignored and the effect of the finite size of the particles and inertia must also be incorporated into the fluid flow equations. In the cases shown illustrated in figures 3-7 and 3-8 we utilized the dense particulate flow in-house code using drag laws that incorporate the effect of the volume fraction and soft sphere inter-particle collision effects:

![Graphs showing evolution of scaled cloud settling velocity and aspect ratio with scaled time.](image)

**Figure 3-7:** (A) Evolution of Scaled cloud settling velocity with scaled time at $Re_c = 11.4$ (B) Evolution of Cloud aspect ratio with scaled time at $Re_c = 11.4$
Figure 3-8: Evolution of scaled cloud settling velocity with scaled time at $Re_c = 14$ (B) Evolution of cloud aspect ratio with scaled time at $Re_c = 14$

As would be expected in the physical process, the cloud responds to gravity by accelerating from zero but due to its horizontal expansion begins to decelerate after reaching a peak velocity.

The DPM simulations used in the work clearly out-performs the Oseenlet simulations used in Pignatel, Nicolas and Guazzelli 26. There are three key reasons for this. First, at the high volume fraction (~0.5) conditions of the simulations and experiment, the drag on the individual particle can no longer be modelled with the straightforward treatment of the stokeslet. The collective motion is stronger due to the slowly decaying $O(1/r)$ interparticle hydrodynamic interactions. Second, the size effects are not accounted for in the stokeslet simulations where the effect of volume fraction is completely ignored. Third, and also as a consequence of the high volume fraction and moderately high Re (~10-14), it is possible that short-range interparticle forces namely the collision dynamics may become significant. Oseenlets do not account for these. However at long time the oseenlet approaches experiments as particle become dispersed and the drag on the particles in the experiment become similar to that of an isolated particle. One may observe that the aspect ratio of the DPM simulations does not grow as fast as that of the Oseenlet despite the fact that the non-linear inertia term is included in the governing equation. There is a brief period between the initialization of the flow and when the blob attains a maximum velocity which is not
captured by Oseenlet simulations. The blob accelerates as a spherical entity in this regime as shown by the simulations but its aspect ratio begins to increase. This causes a greater amount of drag to be experienced by the blob and it consequently begins to slow down.

3.4.2 Particle leakage at low $Re_c$

A spherical dispersion of particles settling under gravity will produce a well-defined tail of particles if the Reynolds number is sufficiently low. Because of the randomness of the leakage process, the process of cloud settling can be termed an irreversible process. For the flow to be considered within the Stokes regime, the criterion used is based on the more stringent $Re_c$ as opposed to the particle based $Re_p$. The random crossing of the imaginary boundary of the blob due to the many-body hydrodynamic interactions allows for such particles to be caught in the background fluid streamlines, swept to the back of the cloud and subsequently lost from the bulk of the cloud. Figure 3-9 shows the streamlines of the fluid flow field at a meridian plane that cuts through the center of the particle distribution.

![Figure 3-9: Particle leakage at low Reynolds Number](image)
Because inertia is almost non-existent in this regime, the particles can no longer catch-up with the rest of the cloud and are lost in an axial tail behind the blob. The streamlines are obtained by plotting the velocity field in a frame of reference that is moving with the settling cloud velocity.

We define a leaked particle as one that fulfills the criterion \( |y_p - \bar{y}| > 1.2R \). The cutoff is greater than the actual radius of the cloud so as to allow for the negligible deviations from the roughly spherical shape of the cloud.

3.4.2.1 Rate of particle leakage and initial particle number

Since particle leakage is a function of the long-range inter-particle interactions, and hence a statistically random process that depends on the configuration and number of particles, we can assume that the rate of particle leakage should be \( f(N_p) \). We studied the leakage of particles with respect to initial particle number. Particles in the simulation are mono-size with \( d_p = 120 \mu m \).

Conditions for the simulations performed are given in Table 3-3. Figure 3-10 shows the time evolution characteristics of the particle leakage process while the rate of leakage extracted from 3-10 is plotted against initial number of particles in the cluster showing exponential relationship between both quantities.

Table 3-3: Parameters for the Particle number parameter study

<table>
<thead>
<tr>
<th>( N_p )</th>
<th>1000</th>
<th>3000</th>
<th>5000</th>
<th>7000</th>
</tr>
</thead>
<tbody>
<tr>
<td>( Re_p )</td>
<td>0.000 300 67</td>
<td>0.000 300 67</td>
<td>0.000 300 67</td>
<td>0.000 300 67</td>
</tr>
<tr>
<td>( \phi )</td>
<td>0.023</td>
<td>0.023</td>
<td>0.023</td>
<td>0.023</td>
</tr>
</tbody>
</table>
Figure 3-10: Particle Leakage with time for various initial number of particles

Figure 3-11: Rate of particle leakage with initial number of particles

3.4.3 Breakup At moderate $Re_c$

There is a qualitative similarity between the breakup-pattern of particle clouds simulated in this work at moderate Reynolds number. The simulation conditions are: $Re_c = 5.0$, $\rho_p/\rho = 2.1$, $St = 0.005266$. Figure 3-12 shows that the DPM simulation is adequate to capture the breakup of the blob into two secondary blobs.
3.4.3.1 Effect of domain shape on cloud breakup

In the simulations carried out, the domain had a square cross-section. For the simulations performed in the Reynolds number parametric study (see section 3.4.3.3), four secondary blobs were produced with consistency indicating that the number of secondary drops produced seems to depend more on the shape of the boundaries than on the Reynolds number of the system. This is slightly different from the findings of Bosse, Kleiser, Hartel and Meiburg 32 who were able to produce different breakup patterns by varying the grid coarseness and the Reynolds number using periodic boundaries for all their simulations. An investigation was also made into the effect of the nature of the boundary conditions and no change in the fundamental pattern of breakup was observed. This is in agreement with the observations outlined by Bosse, Kleiser, Hartel and Meiburg 32. Three boundary configurations were used – the bounded box, fully periodic boundaries, and no-slip boundary conditions in the manner of 35. The bounded box uses periodic boundaries for the vertical walls, fully periodic uses periodic boundaries for all the walls.

Because of the strong dependence of the number of secondary blobs on the shape of the boundaries we can expect 2 secondary blobs to develop in say a rectangular cross-section. The
shape of the domain used in the experiment has a rectangular cross-section and is thus the reason for the amplification of the mode that leads to 2 blobs. This is reproduced in the simulations. We show in other simulations (Figure 3-13) that the number of blobs could be up to 4 where the domain has a square cross section and as many to 6 in the case of a circular domain and all blobs have the same initial conserved quantities. It is concluded that the secondary drops produced are independent of whether the boundaries are impenetrable walls or periodic, what matters is the shape of the boundaries.

We also see that there is no quantitative difference when the domain cross-section used is a square irrespective of the nature of the boundaries by comparing the velocity fluctuations and the aspect ratio evolution for the three types of boundaries. This result has previously been reported for homogeneous sedimentation 35.

Figure 3-13: Effect of nature and shape of boundaries on breakup pattern showing top (top) and side view (bottom)
3.4.3.2 Effect of initial particle distribution on breakup

There is no evidence to indicate that the initial particle distribution has a significant role to play in the secondary breakup pattern. The evolution for an initially random configuration of particles is the same as a regularly spaced distribution of particles. A random number generator was employed to give an initially random particle distribution of the cloud of particles. \( Re_c = 5.0, \ Re_p = 0.00186 \), \( St = 0.0017 \), and \( \rho_p / \rho = 2.1 \) where the initial volume fraction in both simulations was \( \varphi = 0.023 \). Simulations showed a bias to the shape of the boundary than the initial distribution of the particles. The breakup of the cloud produces 2 secondary clouds in keeping with the rectangular cross-section of the domain. This breakup pattern is the same as that produced when the initial particle distribution was a regular square lattice clipped off at the corners to give an initially spherical distribution. We also make a qualitative and quantitative comparison of both cases in figures 3-15 and 3-16 respectively.

It is observed from the results that there is no quantitative or qualitative proof that the randomness of the initial distribution has anything to do with the breakup characteristic of the blob with both having very similar breakup patterns and characteristics. The breakup pattern is thus more a function of the large-scale, hydrodynamic interactions with the boundary and the shape of these boundaries than the isolated individual positions of the particles.
Figure 3-15: Breakup pattern for (A) an initially random (B) Non-random particle distribution

\[ t = 6s \]

Figure 3-16: Comparison of Cloud evolution for initially random and non-random particle distributions (A) Aspect ratio evolution (B) Velocity auto-correlation function evolution

Table 3-4: Comparison of break up quantities of and initially random cloud configuration and non-random configuration of particles

<table>
<thead>
<tr>
<th></th>
<th>RANDOM DISTRIBUTION</th>
<th>INITIAL NON-RANDOM DISTRIBUTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>( t_b(s) )</td>
<td>3.8</td>
<td>3.9</td>
</tr>
<tr>
<td>( l_b(m) )</td>
<td>0.053831</td>
<td>0.054415</td>
</tr>
<tr>
<td>( \gamma_c )</td>
<td>4.01</td>
<td>4.306</td>
</tr>
</tbody>
</table>

3.4.3.3 Reynolds number studies, cloud evolution and breakup

We can quantify the life of the cloud by the break-up time and break-up length. The time between the release of the cloud from rest and the breakup of the cloud into secondary blobs is here defined as the breakup time and the distance travelled is the breakup length which is closely
associated with \( t_{\theta} \). Quantitatively, we define this point as when the aspect ratio of the cloud peaks and then begins to fall as a result of the steady loss of symmetry.

The aspect ratio of the cloud denoted as \( \gamma \) is an important shape characteristic because it quantifies the ratio between the degree of oblation and the degree of prolation. This value affects the effective projected area in the direction of motion of the cloud and directly affects the effective drag seen by the swarm. We calculate this value as square root of the variance of the particle displacement in the \( x \)-direction to the value in the \( y \)-direction. In order to utilize a more robust form of this statistic, the particles that are deemed to have leaked from the blob i.e. particles that are a distance \( >1.20R_{c} \) are not included in the calculation which would otherwise be sensitive to outliers. By defining \( \gamma \) in this way we avoid the arbitrariness of measuring the cloud dimensions based on the furthest particles in each direction.

\[
\gamma = \frac{\sqrt{\sum_{i=1}^{K} f_i \cdot (x_i - \bar{x})^2}}{\sqrt{\sum_{i=1}^{K} g_i \cdot (y_i - \bar{y})^2}}
\]

Pignatel, Nicolas and Guazzelli \(^{26} \) mention that the breakup time is a quantity dependent on only the number of particles in the simulation. It was observed in our simulations that the breakup time and length bear a relationship to \( Re_{c} \).

Figure 3-17 shows how the aspect ratio changes with time for different Reynolds numbers. There is a rapid increase in the aspect ratio at higher Reynolds numbers and the chart is truncated at the moment of break-up where a description of the aspect ratio using equation becomes meaningless. When \( Re_{c} \ll 1 \), the cloud maintains a robust spherical axisymmetric structure and the shape remains a closed spherical cluster.
In order for breakup to occur, a critical aspect ratio $\gamma_c$ must be reached. At this point, the cloud has expanded in the lateral direction into a symmetric, open torus and the higher density cloud forces through the lower density fluid against the stabilizing effect of viscosity. Figure 3-18 shows the point at which this occurs. In the simulations performed we observe that $\gamma_c$ is independent of the Reynolds number of the flow according to table 3-5 and this is so because of the uncertainty that sets in as the flow becomes more chaotic.
Table 3-5: Observed critical aspect ratio for particle cloud settling

<table>
<thead>
<tr>
<th>$Re_c$</th>
<th>$\gamma_c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>3.624912</td>
</tr>
<tr>
<td>5</td>
<td>4.478809</td>
</tr>
<tr>
<td>10</td>
<td>5.099754</td>
</tr>
<tr>
<td>20</td>
<td>5.062558</td>
</tr>
<tr>
<td>30</td>
<td>4.370129</td>
</tr>
<tr>
<td>40</td>
<td>4.62275</td>
</tr>
<tr>
<td>50</td>
<td>4.214646</td>
</tr>
</tbody>
</table>

We plot the breakup time and length respectively against $Re_c$ and find a relationship between both in figure 3-19. From figure 3-20, the breakup time increases asymptotically to $\infty$ as the Reynolds number goes to zero to obtain the following scaling law: $t_b = 8.8749Re_c^{-0.393}$. Also, the non-dimensional breakup length, which is the length travelled by the cloud scaled by the initial radius of the cloud is observed to decrease with Reynolds number and the scaling law obtained is $l_b = 34.338Re_c^{-0.251}$.

![Figure 3-19: Effect of $Re_c$ on (A) breakup time; (B) breakup length](image)

This later result at first seems counter-intuitive because at higher $Re_c$, we would expect that the blob would travel a longer distance in a short time and thus the breakup length should be longer.
However, if we consider that the dispersion of the cloud in the lateral direction means that the effective drag on the cloud increases as it expands and thus reduces the velocity of the cloud. We can observe this by quantifying the expansion of the cloud using the aspect ratio.

3.4.3.4 Velocity fluctuation auto-correlation

One measure of characterizing the evolution of the cloud is to look at the behavior of the VACF with time. This function mathematically correlates the individual velocity fluctuations of the particles with the velocity fluctuation at the beginning of the clouds descent and physically tells us about the hydrodynamic interactions between the particles as they collectively travel in the fluid and the degree of irreversibility of the system. For a fully reversible process in which the viscous dissipation term fully dampens out any distorting effects of inertia on the blob, the velocity correlation should follow a non-decaying, sinusoidal wave in keeping with the Hill’s vortices generated within the cloud substructure. In order to get meaningful results for the velocity auto-correlation function, the suspension cloud should be allowed to reach some steady state. The velocity fluctuations subsequently are then benchmarked against this “steady state”. This places a constraint on the minimum length of the domain. Computational time scales directly as the computational cell count and by extension the computation volume. Simulations of liquid-solid systems have been known to be on the order of one month using other approaches like Lattice Boltzmann simulations \(^{35}\). If the mean particle velocity in a given suspension is given as \( \bar{v}_p = \frac{1}{N_p} \sum_{k=1}^{N_p} v_{p,k} \) time-dependent fluctuation of the particle velocity from this mean \( v'_{p,k} = v_{p,k} - \bar{v}_p \). We can now define the velocity auto-correlation function, VACF as

\[
VACF = \frac{1}{N_p} \sum_{k=1}^{N_p} v'_k(t_0)v'_k(t) \tag{3.8}
\]
In order to study the sensitivity of the evolution pattern of the sedimenting cloud, we observe how the following characteristics change with time: the aspect ratio, the velocity fluctuations and the velocity auto-correlation function of any given system. The key physical property used in changing the Reynolds number was the dynamic viscosity. The initial volume fraction $\varphi = 0.023$ and the density ratio $\rho_p/\rho = 2.1$ were kept constant in all simulations. The simulation domain used had a square cross-section with a dimension of $W/2R_c = 21.806$ with 131,072 hexahedral mesh elements. Boundary conditions used were the impenetrable wall boundary for all six faces of the domain.

Figure 3-20 shows the evolution of the dimensionless average settling velocity for different Reynolds numbers. The three stages of rapid acceleration, self-preservation and dispersion are noticeable in the higher Reynolds numbers. At lower $Re_c$, the acceleration phase and self-preservation phase are longer with $Re_c = 0.1$ showing the highest tendency for self-preservation. This is more noticeable when the velocity auto-correlation function is observed (Figures 3-21 & 3-22).

![Figure 3-20: Normalized average settling velocity of cloud vs. normalized time for different Reynolds numbers](image-url)
3.4.3.5 Evolution of the particle clusters

We present some results for the parameter study we conducted and show that at lower Reynolds numbers, the axisymmetric nature of the cloud is preserved (See Figures 3-23 – 3-25). At moderate to high $Re_c$, the non-linearity of the inertia term becomes dominant and the blob quickly loses its symmetry and breaks up (See Figures 3-26 – 3-28).
Figure 3-23: Shape evolution at $Re_c = 0.1$

Figure 3-24: Shape evolution at $Re_c = 1.0$

Figure 3-25: Shape evolution at $Re_c = 2.0$

Figure 3-26: Shape evolution at $Re_c = 5.0$
Figures 3-27 – 3-28 are the shape evolution when $Re_c$ is moderate. The evolution shows that the mode of dispersion into the host fluid is to go through hydrodynamic instability that causes a loss of symmetry, secondary blob formation and subsequently dispersion.

3.4.4 Interaction among multiple drops

Further verification of the model is provided by exploring the interaction of two spherical particle clouds in comparison to the behaviour of two liquid drops qualitatively. If the discretization of the suspension cloud is fine enough, similarity in behaviour between suspension drops and immiscible liquid drops can be established $^{34}$. The behaviour of two particle clouds (or liquid drops) in an axisymmetric configuration is to create a pressure field around both drops that
causes the leading drop to expand in the horizontal direction and become oblate while the trailing drop expands in the vertical direction and becomes prolate. Figure 3-29 shows the pressure field around a spherical particle configuration where only particles in the meridien plane are shown for clarity. The volume fraction, $\varphi = 0.075$, $\mu = 0.1 Pa - s$, $\rho = 1200 kg/m^3$.

Figure 3-29: Pressure and velocity field evolution of 2 descending, coaxially initialized clouds

The reason for this re-arrangement is that a high pressure stagnation point is setup at the leading end of the both clouds and a low pressure region at the rear. The low pressure region of the leading cloud creates a natural suction for the trailing cloud and deforms it accordingly. The consequence of the rearrangement of particles is an acceleration of the trailing cloud where it pokes through the slower leading particle cloud of the same radius. Leakage results in the trailing particle cloud because as the cloud becomes more prolate, it displays a greater tendency to loose particles in a tail 34.

Two clouds with dissimilar radius also show the same behaviour as two corresponding liquid drops with the leading smaller drop having a tendency to move slower than the trailing larger drop and to “coat” the surface of the trailing drop. This we see in figure 3-30.
Figure 3-30: Comparison between two trailing buoyant drops of different radiiues and two trailing particle clouds of different radiiues in coaxial positions

Particle Cloud interactions in off-symmetric positions are also captured in figure 3-31 and in a more adverse off-symetric position as in figure 3-32. The stagnation point at the leading edge of the trailing cloud and the low pressure region at the tail end of the leading cloud creates a natural suction for the distortion of both clouds.

Figure 3-31: Comparison between two trailing drops of different radiiues and two particle clouds of different radiiues in off-symmetry positions

Figure 3-32: Comparison between two trailing drops of different radiiues and two trailing particle clouds of different radiiues in accentuated off-symmetry positions
As has been discussed in the preceding section, the motion of a cluster of particles in the wake of another particle cluster would cause an increase in the settling speed of the trailing cluster. It would also cause changes in the structural properties of the cluster. We examine the dynamics of the two particle clusters in axial flow in two specific scenarios: First, when the particles in the trailing cluster have a density half of those in the leading particle cluster; second, when the particles in the trailing cluster have a density double the leading cluster. In order to examine the structure, we use the transverse (x-direction) Root Mean Square (RMS) position of the individual particle clusters and the Axial (in the direction of flow) skewness (Skew). The RMS gives us the spread of the cluster of particles in the transverse direction while the skewness in the y-direction gives us the deviation of the distribution of particles from a symmetric distribution. A low value for the skewness (negative) means more particles are concentrated on the leading front of the cluster while a high value means the particles are concentrated to the rear in the direction of flow. The definition of the RMS particle position is given in equation 3.9 while the skewness is given by equation 3.10

\[
RMS = \sqrt{\frac{1}{N} \sum_{i=1}^{N_{bins}} f \cdot (x_i - \bar{x})^2}
\]  

(3.9)

\[
Skew = \frac{1}{N} \sum_{i=1}^{N_{bins}} f_i \cdot (x_i - \bar{x})^3 \left( \frac{1}{N} \sum_{i=1}^{N_{bins}} f \cdot (x_i - \bar{x})^2 \right)^{\frac{3}{2}}
\]  

(3.10)

3.4.4.1. Heavy cluster leading, light cluster trailing

Figure 3-33 shows results for a simulations with the leading cluster having the following properties: \( Re_c = 1.25 \), \( Stk = 4.4E - 4 \), \( \rho_p/\rho = 2.5 \) and \( \varphi = 0.05 \). The trailing cluster has the following properties: \( Re_c = 0.42 \), \( Stk = 8.7E - 5 \), \( \rho_p/\rho = 1.5 \) and \( \varphi = 0.05 \)
We label the plot on the right hand side of figure 3-33 to highlight various structural changes that take place in the particle cluster configuration. At point 1, the heavier cluster is at its lowest skewness indicating particle concentration at the rear of the cloud. And the corresponding picture of the cluster shows that the cluster has a spherical dome shape. At point 2, the trailing cluster extends into the wake of the leading cluster but also has a higher concentration of particles at the rear. At point 3, the particle cluster structure has almost recovered its initial spherical configuration while the trailing cluster recovers slowly. At point 4, the heavy cluster regains a negative skewness for a short time before the cluster eventually begins to leak particles indicated by an increase in skewness. Meanwhile, the RMS plot of the process shows a very simple behavior.
when a heavy particle cluster is leading a lighter particle cluster. The RMS increases for the leading cluster indicating greater transverse dispersion while the RMS decreases for the trailing cluster indicating less transverse flow. The effect of the modification of the structural properties of the trailing cluster of particles brings about an upward modulation of the velocity of the as shown in figure 3-34 where we compare to a single particle cluster of same properties.

![Figure 3-34: Enhancement of vertical velocity of trailing, light cluster](image)

In figure 3-34 the particle velocity increases sharply for the trailing cluster over an isolated one but saturates due to expansion in the lateral direction and an attendant increase in drag.

### 3.4.4.2. Heavy cluster trailing, light cluster leading

Figure 3-35 shows a much different picture when the particle clusters are reversed in position. The properties are the same as in the previous section.
An observation of the RMS position of the particles in the transverse direction shows that the leading lighter particle cluster expands rapidly in the transverse direction to make way for the trailing heavier particle cluster. The heavier trailing cluster conversely has a reducing RMS until point 3 in the figure 3-35 and then begins to recover as it pushes past the leading lighter cluster. The RMS of the lighter cluster then reduces because it is now caught in the wake of the heavier cluster and is forced to contract in the lateral direction. The evolution of the skewness in the direction of shows that the heavier cluster loses particles in its tail from point 1 onwards as shown by the increasing skewness.
As is shown in figure 3-36 the draft provided by the leading particle cluster causes an increase in the velocity-time profile of the particle cluster from an isolated cluster to one in the draft of another particle cluster. The kink in the higher curve at around 1500 time units would indicate the point when the pressure gradient that exists between the leading and the trailing particle cluster is highest and provides resistance to the motion. Once the cluster of particles has proceeded past the leading cluster, it begins to expand in the transverse direction and the velocity reduces due to increased drag force.

3.5 Conclusions

The sedimentation of a cloud of particles in a viscous fluid at low and moderate Reynolds numbers has been studied. We looked at the volume fraction dependence of the settling cloud and find a similar dependence in the simulations as in the theoretical predictions of 1. The average cloud settling velocity and the velocity fluctuations around this average are found to have a linear dependence on $\phi^{1/3}$ at negligible Reynolds number. The velocity fluctuations display strong
anisotropy with the magnitude of the vertical component almost three times the magnitude of the horizontal component.

At high volume fractions, and moderate Reynolds numbers, particle-particle interactions become important and a drag law that accounts for the finite volume of particles is required in the modeling.

Similarities in the interaction between a system of two particle clouds and a system of two immiscible droplets was established with an observed increase in the velocity of the trailing cloud due to drag reduction in the wake of the leading cloud. The formation of the stagnation points at the leading front of the cloud is pointed to as the cause of shape deformation in these systems. Particle leakage at low Reynolds number was established and found to be directly related to the initial number of particles.

At higher Reynolds numbers, the cloud of particles evolved into an open torus and subsequently loses its axi-symmetry and breaks-up into a number of secondary clouds. This process is a type of Rayleigh-Taylor instability and the number of secondary drops was found in our simulations to be dependent on the shape of the boundaries used rather than the nature of the boundaries.

Breakup at moderate $Re_c$ is found to occur after a critical aspect ratio is reached and a scaling was proposed for dependence of the breakup length and breakup time on $Re_c$. It may be necessary in future works to find the dependence of the critical aspect ratio on the number of particles in the particle cloud.
Chapter 4 Simulation of Gas-Solid Flows in a Small-Scale Fluidized Bed Using a Newly Developed Momentum Interphase Drag Coefficient

4.1 Introduction

Volume averaging of the Navier-Stokes equation presents a convenient way of treating multiphase flow systems where direct numerical modelling approaches prove time-consuming and costly. The upshot of the averaging however is a loss of information since the magnitude of the skin and form drag around individual particles is lost during averaging\(^{58-60}\). Traditionally, the resulting extra terms for which appropriate closures must be found have been grouped into three categories according to Jackson\(^{11}\): those that depend on relative velocity of the phases (drag), those that depend on the relative acceleration of the phases (virtual mass force) and those that are normal to the direction of the drag force (lift forces). The virtual mass force and the lift forces both depend on the ratio of the density of the continuous phase to the density of the dispersed phase and are for all intents and purposes negligible in gas-solid systems\(^{61}\). The most important of these is therefore the drag force for which various approaches have been explored to define the closures relationship. The method of providing these closures either come from empirical observations of pressure drop across packed or expanded beds\(^{62-64}\) or sedimentation of a suspension of particles\(^{65}\), analytical techniques\(^{66,67}\) and particle-resolved-type models like Lattice Boltzmann simulations\(^{68}\).

Wilhelm and Kwaak\(^{69}\) present some of the earliest work to try to quantify fluidization behavior using a Froude Number \((Fr_{mf} = u_{mf}^2 / gd_p)\) based on the minimum fluidization velocity. If \(Fr_{mf} \ll 1\) the fluidization is uniform, homogenous and the height of the bed should bear a linear relationship to the flowrate of fluid through the bed. The vast majority of these closure relationships are adequate for homogeneous (solid-liquid) fluidized beds where the Froude number
of the fluidized bed is sufficiently small \(^{70}\). The application of such drag laws to modeling gas-solid fluidization where \(Fr_{mf}\) is 100 order of magnitude greater than liquid solid fluidized beds may result in unsatisfactory prediction of the pressure gradient across the bed even if the time-averaged overall pressure drop equals the weight of the bed. It should hence be pointed out that while the overall pressure drop is a function of the weight of particles in the bed, the pressure gradient across the bed is a function of the velocity-voidage relationship. This is not a trivial picture as the regime of fluidization as governed by \(Fr_{mf}\) gives rise to coherent inhomogeneous structures including bubbles, slugs and clusters hence the need to cast the simulation of gas-solid systems as a multi-scale problem with different length and time-scales \(^{71, 72}\). As a consequence of the use of inappropriate drag laws, the pressure gradient across a fluidized bed is often over-predicted by existing drag models \(^{73}\).

Vejahati, Mahinpey, Ellis and Nikoo \(^{73}\) attempt to improve the accuracy of the drag coefficient by proposing an objective function that satisfies the following equation \(U_{mf} - Re_{ts} \left( \frac{\varepsilon \mu}{p_d_d_p} \right) \to 0\). Other efforts have been made to account for the effect these inhomogeneous structures have on the drag relationship within bed. The most famous put forward by Li \(^{74}\) where a multi-scale model is put forward for correctly modeling the drag in a gas-solid fluidized bed with coherent meso-scale structures. They cast the drag as an optimization problem with eight input parameters (four each for the dense and dilute particle phases) that include volume fraction, velocity field, the particle diameter and particle radius with the objective of minimizing the energy dissipation in the bed. This is perhaps the best known method for correctly resolving issues with over-prediction of the pressure drop in non-particulate fluidization but may suffer from increased numerical costs due to additional numerical calculations devoted to optimizing for \(C_D\).
No single drag law may be universal enough in capturing the entire regime map of fluidized bed operation. Whatever scheme we use for estimating the drag (and hence the pressure drop) must respect energy conservation by balancing the Power input as a function of inlet flow rate to the average head of the bead and the energy dissipation rate due to the presence of particles.

4.2 Simulation method

The discrete element method coupled with computational fluid dynamics is used in modeling the case studies in this work. We solve the continuum phase equations using the finite volume method and tracking the discrete phase explicitly through particle dynamics. The benefit of using a DEM-CFD approach is that assumptions need not be made about particle stresses and dispersed phase boundary conditions do not need to be estimated from phenomenological models. These are calculated directly and discretely per particle contact using any of the existing soft-sphere contact models. For fluidized beds 2-way coupling is reflected in the calculation of the drag terms. Particle-Particle interactions are modelled using a soft sphere viscoelastic Hertzian model. DEM-CFD mathematical models popularized by Tsuji, Kawaguchi and Tanaka and Hoomans, Kuipers, Briels and vanSwaaij have previously been explained in section 2.3.2.

Pressure-Velocity coupling is handled by the SIMPLE Algorithm and 3rd order spatial discretization is employed for the momentum terms using QUICK scheme and 2nd order spatial discretization for pressure.

4.3 Closure models

In order to calculate interphase momentum coefficient as expressed in table 1, we employ descriptions put forward by Gidaspow in equations 4.1 and Syamlal, Rogers and O’Brien in equations 4.2.
Gidaspow Model:

\[
\beta_{\text{Gidaspow}} = \begin{cases} 
\beta_{\text{Wen\&Yu}}, & \varepsilon_s < 0.2 \\
\beta_{\text{Ergun}}, & \varepsilon_s \geq 0.2 
\end{cases}
\]  

(4.1a)

\[
\beta_{\text{Wen\&Yu}} = 3C_{D,\text{WY}} \frac{\varepsilon_s \rho}{d_p} |u - u_p| \varepsilon^{-2.65}
\]  

(4.1b)

\[
C_{D,\text{WY}} = \begin{cases} 
\frac{6}{Re} (1 + 0.15 Re^{0.687}), & Re \leq 1000 \\
0.11, & Re > 1000 
\end{cases}
\]  

(4.1c)

\[
\beta_{\text{Ergun}} = 150 \frac{\varepsilon_s^2 \mu}{\varepsilon d_p^2} + 1.75 \frac{\varepsilon_s \rho}{d_p} |u - u_p|
\]  

(4.1d)

Syamlal Model:

\[
\beta_{\text{Syamlal}} = \frac{3 C_{D,\text{SYAM}} \rho}{4 f^2} \frac{|u - u_p|}{d_p} \varepsilon \varepsilon_s
\]  

(4.2a)

\[
C_{D,\text{SYAM}} = (0.63 + 4.8 \sqrt{f/Re})^2
\]  

(4.2b)

\[
f = 0.5 \left( A - 0.6 Re + \sqrt{0.06 Re^2 + 0.12 Re (2B - A) + A^2} \right)
\]  

(4.2c)

\[
A = \varepsilon^{4.14}
\]  

(4.2d)

\[
B = \begin{cases} 
\varepsilon^{2.65}, & \varepsilon_s < 0.15 \\
0.8 \varepsilon^{1.28}, & \varepsilon_s \geq 0.15 
\end{cases}
\]

4.3.1 New drag model

The drag seen by a particle in a fixed or expanded bed is easily related to the pressure drop. Equation (4.3) expresses the drag coefficient as a function of the particle Reynolds number, \(Re_p\) and the local voidage and solid hold-up, \(\varepsilon\) and \(\varepsilon_s\)

\[
C_D = \frac{6}{Re_p} \left[ \frac{3.6 \varepsilon_s}{\varepsilon^4} + 1 \right]
\]  

(4.3)

A complete derivation of equation (4.3) can be found in Pandit and Joshi \(^{78}\) while a brief summary is given in Appendix B. Its derivation begins with the Hagen-Pouiseuille equation for the pressure drop in a straight tube. By using the equivalent diameter of cross-sectional area
available to flow and surface area exposed to flow in a bed of particles, the pressure drop due to skin friction is related to the volume fraction. The pressure drop due to form drag is derived from the tortuosity and added to the skin drag to arrive at the overall pressure drop across the bed in a laminar regime. This pressure drop for the entire volume of the bed is related to the volume of a single particle and the expression for the laminar portion of the drag coefficient for the particles is derived.

The turbulent portion of the drag coefficient is expressed as:

\[ C_D = 0.11 \left( \frac{40.91 \varepsilon^2}{\varepsilon^2 + 1} \right) \approx 0.11 \varepsilon^{-4.8} \quad (4.4) \]

A complete derivation of equation (4.4) is also given in Joshi.\textsuperscript{67} At equilibrium, the energy input rate into the bed is balanced by the energy of fluid leaving the bed and the net power dissipation in the bed. Using this energy balance we can estimate the energy dissipation in the bed. Also, we can employ the force balance around a single particle to express the drag coefficient as a function of the energy dissipation. Equations (4.3) and (4.4) are added together to give a drag law that transitions between the laminar and turbulent regimes.

One assumption made in deriving (4.4) is that the scale of turbulence is approximately equal to half the particle diameter. If we express (4.4) in the form of an Ergun friction factor we obtain (3).

\[ f = 0.33 \varepsilon^{-1.8} \quad (4.5) \]

For the case of a fixed bed of particles where \( \varepsilon = 0.4 \), \( f \) works out to be 1.72. By comparison, the coefficient of the turbulent part of the Ergun equation is 1.75. \( \varepsilon \) is not in every
part of the bed equal to 0.4 hence usage of the Ergun equation component without modification for expanded beds may be inaccurate.

Second, and very importantly, proper account must be made for the heterogeneities that exist in the form of bubbles (regions of large void fractions), and slugs in gas-solid fluidized beds. The non-uniform and dynamic nature of the flow structures are accounted for in the adjusted drag law we propose according to equation (4.6) and is used in place of equation (4.4).

\[
C_{D, Adjusted} = 0.11 \left[ \frac{40.91(K\varepsilon_s)^2}{\varepsilon^2} + 1 \right] \tag{4.6}
\]

\(K\) is the adjustment factor that accounts for the amount of energy in the input fluid stream used in sustaining the extra potential energy head of the bubbles and is defined in equation (4.7).

\[
K = \frac{u_{mf}}{u_{inlet}} + \left(1 - \frac{u_{mf}}{u_{inlet}}\right) \left(1 - \frac{\varepsilon_s}{\varepsilon_{s,mf}}\right) \tag{4.7}
\]

In the limiting case of a bed close to the minimum fluidization velocity, \(K\) reduces to 1. This is significant because a combination of equation (4.3) and (4.6) gives a form that looks like the Ergun component of the Gidaspow Drag Equation and also if we compare to the Wen and Yu component of Gidaspow we also see the similarity between the 2 models. We show the comparison between this new model and the Wen and Yu model in Appendix B as well. What the factor \(K\) gives is an extra parameter to reduce the drag for particles in a bubbling-slugging fluidized bed and consequently a smaller pressure gradient and lower hold-up profile. The full derivation of equation (4.6) is given in appendix B. Equation (4.6) is combined with equation (4.6) to give an expression for drag as it transitions between laminar and turbulent regime. It also reduces to a drag law suitable for estimating force on isolated, single particle.
In order to test the validity of the adjusted drag law, we benchmark against experiments and compare with 2 widely used drag models – Gidaspow model \(^{77}\) and Syamlal et al. model \(^{64}\) (referred to as Syamlal for the rest of the paper) – and use them to simulate a bubbling fluidized bed as described in the 2013 National Energy Technology Laboratory (NETL) Small-Scale Challenge Problem (SSCP).

The geometry simulated is shown in figure 4-1. For a more detailed description of the apparatus we refer the reader to the NETL-DOE SSCP available at their website. First and second order moments for the Pressure time series and the transverse velocity profile are compared to results from the experiment.

![Figure 4-1: Geometry for the fluidized bed](image)

Parameters used in the simulation as given by the National Energy Technology Laboratory are given in table 4-1.
### Table 4-1: Computation Parameters

<table>
<thead>
<tr>
<th>Particles</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density</td>
<td>$1131kgm^{-3}$</td>
</tr>
<tr>
<td>Diameter</td>
<td>3.256mm</td>
</tr>
<tr>
<td>Minimum fluidization velocity ($u_{mf}, m/s$)</td>
<td>1.095</td>
</tr>
<tr>
<td>Superficial gas velocity</td>
<td>$2u_{mf}, 3u_{mf}, 4u_{mf}$</td>
</tr>
<tr>
<td>Particle Count</td>
<td>~95,000</td>
</tr>
<tr>
<td>Normal restitution coefficient, p-p collisions</td>
<td>0.84</td>
</tr>
<tr>
<td>Tangential restitution coefficient, p-p collisions</td>
<td>0.65</td>
</tr>
<tr>
<td>Coefficient of Friction</td>
<td>0.35</td>
</tr>
</tbody>
</table>

### Computation

| Inlet boundary condition          | Velocity Inlet             |
| Outlet boundary condition        | Pressure outlet            |

### Spatial Discretization

| Pressure                          | Standard                  |
| Momentum                          | QUICK                     |
| $\Delta t_{fluid}$                | 0.001s                    |
| $\Delta t_{DPM}$                  | 0.00002                   |

### 4.4 Results

Figures 4-2, 4-5, 4-8 provide the profiles of the particle distributions in a slugging fluidized bed for the different superficial gas inlet velocities given in table 4-1. The particles are colored by the velocity magnitude. The Gidaspow drag relationship is used in simulating this case. For other drag laws employed in this work, the picture remains roughly similar.

Immediately apparent is the complex bubbling-slugging nature of the fluidized bed and the dynamic nature of the bed height. Due to high aspect ratio, there is a preponderance of slugs as opposed to bubbles. This is strongly inhomogeneous behavior is typical of the flow Geldart D classification of particles in high aspect ratio beds where bubbles rise less quickly than the interstitial gas such that gas flow is into the bubble and out at the top, rupturing the bubble. Because this gas flow at $4u_{mf}$ is very rapid, and the bed is thin, the flow of gas into the gas ‘bubbles’ is sufficient for the bubbles to be stretched into slugs.
Figure 4-3, 4-6 and 4-9 show the time-averaged solid phase horizontal velocity for the three inlet velocity cases where inlet velocity of the gas is uniform at $2u_{mf}$, $3u_{mf}$ and $4u_{mf}$ respectively. The profile is for an iso-surface that slices through the middle of the geometry.

The solids horizontal were averaged over 20s at a sample rate of 1000Hz. The three profiles shown are for the three drag laws employed in this study. The result primarily show that despite the very dynamic and rapid nature of the fluidized bed and the 1-D nature of slugs in beds of high aspect ratio, there is a clear 2-D quasi-steady transverse circulation cells of the particles. The Gidaspow and Syamlal models show much similarity in terms of the height to which the circulation cells reach, however, the profiles for the adjusted drag law we have developed show the circulation cells to be less than those for the traditional drag laws. This is due to the reduction in the magnitude of the drag as provided for by the drag law introduced.

Figures 4-4, 4-7 and 4-10 show the time-averaged solid phase vertical velocity for the three cases earlier described. It is averaged at a sample rate of 1000Hz. It tells the same story as Figures 4-3, 4-6 and 4-9. Circulation cells of particles have been established. The particles rise through the central portion of the tube where resistance to gas motion is lowest due to a lower hold-up and fall along the sides of the tube. We also see that in comparison to Gidaspow and Syamlal models, the highest velocity reached by the particles at 0.172m/s as predicted by our adjusted drag model is much lower than the highest velocity predicted by the Gidaspow and Syamlal models. This again is attributable to the lower magnitude of the interphase drag term for the proposed drag adjustment. We draw this conclusion by considering that the input of mechanical energy into the bed as a result of inflow of the gas goes into sustaining not only the potential energy of the bed but also the kinetic energy used up in the flow of gas and particles and the energy dissipated due to drag around each of the particles.
Figure 4-2: Complex bubbling-slugging regime at inlet velocity of $2u_{mf}$
Figure 4-3: Time-averaged horizontal solid velocity profile at inlet velocity of $2u_m f$ for the 3 drag models used.

Figure 4-4: Time-averaged vertical solid velocity profile at inlet velocity of $2u_m f$ for the 3 drag models used.
Figure 4-5: Complex bubbling-slugging regime at inlet velocity of $3u_{mf}$
Figure 4-6: Time-averaged horizontal solid velocity profile at inlet velocity of $3u_{mf}$ for the 3 drag models used

Figure 4-7: Time-averaged horizontal solid velocity profile at inlet velocity of $3u_{mf}$ for the 3 drag models used
Figure 4-8: Complex bubbling-slugging regime at inlet velocity of $4u_{mf}$
Figure 4-9: Time-averaged horizontal solid velocity profile at inlet velocity of $4u_{mf}$ for the 3 drag models used

Figure 4-10: Time-averaged horizontal solid velocity profile at inlet velocity of $4u_{mf}$ for the 3 drag models used
One consequence of adjusting the drag downwards is that in principle, the pressure gradient should also be adjusted downwards. In Figure 4-11 we show the pressure drop for three cases and for the different drag laws.

Figure 4-11: Time-averaged axial pressure drop between z=0.0413m and 0.3641m. Curve 1 uses Gidaspow, 2 uses Syamlal, 3 uses the new drag law and 4 corresponds to experiments.

The pressure drop shown is the time-averaged value of pressure drop over taps as shown in the schematic in figure 4-1 across an axial length between a depth of 0.0413 and 0.3461m. The sampling rate is 1000Hz. We see that for case 1, the pressure drop as predicted by all three models are different from the experimental value by about 10% in both case 1 and case 2. However in case 3 the difference between the pressure drop predicted by Gidaspow and Syamlal models becomes well over 35%. However, using the new drag relationship developed in equation 4.6, better agreement between the simulations and the experiments is achieved. This is also seen when we consider the second order moments of the pressure drop as shown by the rms pressure across the same taps in figure 4-1. The simulated rms pressure drop produces excellent agreement with the experimental rms pressure drop in comparison to the other closure models. This essentially means that the magnitude of the fluctuations of the pressure drop estimated by our new drag law is
comparable to those in the real experiment. This is due to the attenuation of the energy dissipation in the bulk gas around the particles by accounting for the energy required to sustain the extra energy head due to bubbles and inhomogeneous structures. As will be seen shortly, the procedure adopted in estimating the drag around the particles also has consequences on the frequency of oscillation of the pressure drop across the bed.

Figure 4-12: RMS axial pressure drop between $z=0.0413m$ and $0.3641m$. Curve 1 uses Gidaspow, 2 uses Syamlal, 3 uses the new drag law and 4 corresponds to experiments

Figure 4-13 shows the times series of the pressure fluctuations less the time-averaged pressure drop across the taps for case 1 where the velocity at the inlet is $2u_{mf}$. A common view is that the pressure signals as a measure of the hydrodynamic state of the bed include effects of gas turbulence, gas bubble/slug formation and bubble/slug eruption. The strong fluctuations in pressure time series indicate the highly dynamic nature of the bed and the motion of pressure waves through the bed. The right hand side of figure 4-11 shows the Fourier transform of the time-series of the pressure drop where the magnitude of the amplitude of the pressure fluctuations are plotted against the frequency of fluctuations. The bandwidth for presenting the spectral analysis is 50Hz (we show up to 10Hz). We see that the dominant frequency for the simulations using the Gidaspow
and Syamlal models lies around 3.25Hz while the dominant frequency for the adjusted model is 2.7Hz. The adjusted model thus shows closer agreement to the experiment whose dominant frequency is determined to be 2.5Hz. Again, the reduction in the frequency of fluctuation is also determined by the magnitude of the drag used in modelling particle-fluid interactions.

Figure 4-13: Time-series and Fourier transform of the pressure drop signal for the simulated cases and experiments
Finally, a comparison between the proposed drag law and existing drag relationship is shown in figure 4-14 a comparison of the various velocity profiles as shown using the Gidaspow and Syamlal models the current model and experiments.

Figure 4-14: Time-averaged transverse vertical solid velocity profile at z=0.076m. 1 is using Gidaspow, 2 Syamlal, 3 the new drag law.

We observe that due to the tempered drag prediction, area under the velocity profile curve for the adjusted drag relationship is lower than that for the existing drag laws and the quality of the prediction is not degraded when comparing to the experimental values.

One consequence of controlling the interphase drag is the reduced height of the bed of particles. This we see from figure 4-15 where the axial solids volume fraction profile is plotted against position. In all cases, the height of the bed of particles as predicted by the adjusted drag law is less than what is predicted using the Gidaspow and Syamlal model.

Figure 4-15: Axial solid holdup profile for 3 inlet flow rates predicted by Gidaspow (curve 1), Syamlal (curve 2) and the current drag law (curve 3)
4.5 Conclusions
We have derived from macroscale energy balance arguments an adjusted drag law for the prediction of behavior of a bubbling/slugging fluidized bed under 3 inlet conditions. We compared the performance of the drag we derived to the performance of the Gidaspow model and the Syamlal model and benchmark our results against experimental values. We find that for intense bubbling and slugging behavior in a fluidized bed, the magnitude of the drag as predicted by existing drag laws may often be over-estimated and yield in higher than expected prediction of the pressure drop. An adjustment of the drag model by accounting for the extra head required in sustaining the expanded bed height due to bubbles and slugs may be needed in attenuating the pressure drop. This has the added effect of making the tempering the particle velocity profile and bring agreement with experiments.
Chapter 5 A Discrete Element Method Study of Granular Segregation in a Circular and Non-Circular Rotating Drums *

5.1 Introduction

The study of the behavior of a dense collection of particles in a rotating drum is not a new pursuit. Nevertheless, the rich parameter space and large number of phenomena observed in these systems give rise to many interesting open questions in the field. Of particular interest in this work is the behavior of a bed of particles in a rotating drum. The impact of discrete entities in the form of particles in granular systems gives rise to many phenomena that are much different from their fluid counterparts despite the fact that the system size may be many orders of magnitude larger than the particle. And the phenomena are counter-intuitive based on our knowledge of continuum fluid mechanics. For instance, if a granular system containing particles of certain density and size combinations is agitated, the tendency is for the mixing entropy to reduce rather than increase. Conversely, a multicomponent mixture would have an increased mixing entropy if agitated 9.

When a mixture of granular materials is sheared there is a tendency for some form of separation to occur 81. Rosato, Strandburg, Prinz and Swendsen 82 show that upon agitation of a mixture of nuts, larger (Brazil) nuts rise to the top with the smaller ones settling to the bottom. Savage and Lun 83 explained the segregation of granular materials by attributing it to small size particles falling through a dynamic sieve, the sieve being the interstitial void spaces provided by larger particles. They also proposed a squeezing mechanism that relies on the force imbalance on individual particles of different properties in the vicinity of other particles. Bridgwater, Foo and Stephens 84 had earlier defined a percolation velocity for the small sized particles.

---

* This chapter appeared as O. Ayeni, C. Wu, J. Joshi and K. Nandakumar, Powder Technology 283, 549-560 (2015)
The question of segregation in rotating equipment which provide a continuous source of exposure of the surface of particles to gravity and thus shear were reported by Nityanand, Manley and Henein\textsuperscript{85} who studied the size segregation in ball mills and scaled up the equipment by using two dimensionless quantities, the Froude number and the size ratio of particles. Ristow\textsuperscript{86} looked at density segregation in a two dimensional rotating drum and followed the inwardly spiraling trajectory of heavier particles. Other examples of segregation have appeared in the literature: axial segregation where alternating bands of particles with a definite wavelength are formed as a result of differences in particle wall interaction and internal angles of repose\textsuperscript{87}, occurs long after radial segregation\textsuperscript{88} and through the coarsening of axial bands\textsuperscript{9}; Drahun and Bridgwater\textsuperscript{89} show alternating layers of particles when a mixture of granular material is poured into a heap.

The bulk of studies of granular dynamics in non-circular shaped geometries have already been carried out with many focusing on pattern formation\textsuperscript{90-94}. We will present a few results for validation purposes, where we are able to reproduce some interest patterns in granular systems while also providing our own take on quantitative assessment of the segregation.

Also of interest has been the means to properly model granular systems. Khakhar, McCarthy, Shinbrot and Ottino\textsuperscript{95} employed a heuristic continuum model to describe the mixing process in a circular tumbler building on earlier descriptions of the velocity profile of the continuous flowing layer\textsuperscript{96, 97}. By conducting a balance of fluxes, they were able to extract expressions for an effective particle diffusivity. Other models that have been employed to study mixing and segregation include Monte Carlo methods\textsuperscript{82} and kinetic theory models\textsuperscript{98} which predict the flux of smaller particles to regions with higher granular temperature and those of larger particles to lower granular temperature regions. Two-dimensional molecular dynamic simulations have also been applied to study size driven segregation\textsuperscript{99}. A review of these methods has been
undertaken by Ottino and Khakhar. In the present work, we will use the particle dynamic, better known as Discrete Element Method simulations as a primary tool of investigation.

5.2 Simulation procedure

The governing equation for the granular system is Newton’s law of motion for a rigid body. The net contributions of long-range (gravity) and short-range (inter-particle and particle-wall forces) is used to calculate the acceleration, advance velocity and advance position using a simple kinematic equation.

The particle mass is $m_i$ while its velocity is $u_i$. The first and second terms on the rhs of equation (2.24) represent the far-field pressure gradient and the drag force exerted on the particle by the fluid and together represent all the forces acting on the particle by the fluid phase. Because the momentum of the gas phase in such systems is negligible and the order of magnitude difference in the inertia of the particle to the air is $\sim 10^3$, we can to a reasonable extent ignore the particle-fluid forces in the implementation of the governing equation without loss of quantifiable detail.

Also, to preserve the six degrees of freedom, the rotational component of the motion of particles is also taken into account:

We use the viscoelastic, Hertzian model in describing particle-particle interactions. DEM time-step satisfies the condition $\Delta t_{DPM} \ll 2\pi \sqrt{\frac{m}{k}}$ in order to properly resolve the soft sphere dynamics of the particle interactions – $m$ is the effective mass of two particles in contact.

Domain decomposition is used for parallelization while multithreading is used to achieve optimum load balance. In calculating the contact forces, a linked-cell algorithm is employed as described by Wu, Ayeni, Berrouk and Nandakumar. Potential particle contacts are detected by
scanning cells in the immediate vicinity of a test particle and all particles residing in such cells are linked to the test particle in a linked-list.

In order to simplify the computation, we can take advantage of the regime of tumbler operation we find ourselves. Since the motion is in the active layer of particles only, and the bed of particles is fixed relative to the walls, we can redefine acceleration due to gravity, \( g \) such that it depends on the angular velocity. This is important since the layers of particles within the bed in the region of the walls has zero velocity in the rotating reference frame of the domain. A comparison between this solution approach and the explicit prescription of the wall velocity will not result in the degradation in the quality of the results.

5.3 Regimes of transverse flow in tumbler operation

Depending on the speed of rotation of the tumbler, there are a number of regimes that have been identified: the avalanche regime (rolling), the cataracting regime and the centrifugal regime.

\( Fr \) is a key dimensional parameter that governs regime transition. Tjakra, Bao, Hudon and Yang mention that the tumbler operating regime should be guided by the process required to apply it to. In grinding for instance where particle collisions are important we may want to use the tumbler in the cataracting regime. A centrifuging regime does not allow for collisions as much.

Figure 5-1 shows the progress of an initially separated bed of particles where both particles have the same properties. \( Fr = 0.0027 \) indicating that gravity dominates centrifugal forces. In all cases the tumbler is impulsively started at the rotating velocity.
Figure 5-2: Cataracting Regime, Fr=0.7339

In the Rolling Regime, the gravitational forces dominate the flow. If the motion is started impulsively from zero rotational velocity, the entire bed remains a static bed in passive rotation. That is, there is no relative angular motion between the bed and the walls of the tumbler. This motion continues until the bed reaches the natural angle of repose of the material. The angle of repose is primarily related to the coefficient of friction. It is worth mentioning that other parameters for the particles like the Poisson ratio, Young’s modulus and particle density do not affect the angle of repose. Once the angle of repose is exceeded, the particle starts to flow across the air-grain interface in a thin, dynamic layer. We will show subsequently how segregation and mixing in the rolling regime takes place in this dynamic layer and how chaotic complexity may bring about improvement of mixing and segregation. When gravitational and centrifugal forces are of the same order magnitude, cataracting regime ensues as in figure 5-2.
This occurs when particles begin to detach from the wall of the containing vessel and the surface of the bed and are flung into the air. Since the centrifugal and gravitational forces are comparable in magnitude, the bed of particles maintains an equilibrium “S”-shape as shown in figure 5.2. This regime also produces rapid mixing of the particles.

When centrifugal forces become an order of magnitude higher than gravitational forces, the particle bed becomes “smeared” on the surface of the tumbler until an equilibrium state is reached where the entire tumbler periphery is coated with layers of particles, depending on how many particles were initially in the bed. This is shown in figure 5-3. While various regimes provide interesting dynamics for study, we will narrow our focus to behavior under rolling regime of tumbler operation.

Figure 5-3: Centrifuging Regime, Fr=4.5872

5.4 Mixing and segregation phenomena attributable to the rolling regime of tumbler operation

The process of mixing in rotating drums involves two processes: a convection-like process where the mixing is driven by the bulk motion of the drum and a random diffusion-like process due to microscopic migration of particles due to inter-particle interactions. Bulk mixing is dominant in the transverse direction while diffusional mixing is apparent in the longitudinal direction where the effect of bulk mixing is non-existent. The concern is that rotary drum

102
simulations contain a mixed bag of parameters but the focus has been on the large scale driving forces: Centrifugal force and gravity.

As a preliminary validation, we carried out simulation to investigate pattern formation in the rolling regime. The system studied here is the rotating drum in the rotating regime as described in Ottino and Khakhar\(^{100}\). Figure 5-4 shows good agreement between the simulations in the rolling regime and experimental results. Previously the simulations were carried out using a phenomenological model that divided the particle motion into both diffusive and convective part and included a diffusion term in the particle motion.

![Figure 5-4: Comparison Between pattern formation in rotating tumbler in simulations and experiments\(^{100}\).](image_url)

There are many characteristics that differentiate granular flow from fluid flow. For instance when particles with different densities or size that are initially well mixed are tumbled, they separate into radial layers of particles with the larger or less dense particles at the periphery and smaller or more dense particles at the center. This provides one example where the addition of energy in the form of mechanical work leads to a decrease in the entropy of mixing (in a granular sense) as opposed to the increase in entropy when two miscible fluids are stirred. It is possible that the entropy of a granular system of 2 particle species can increase, but care has to be taken in
selecting the right density ratio and size ratio that would lead to mixing. Figure 5-5 is the qualitative picture of particles in the tumblers after less than one revolution at 0.21 rads$^{-1}$. The small red particles are the steel beads which have half the diameter of the blue colored glass spheres. The depth of the tumbler is 3 times the diameter of the larger particle.

![Figure 5-5: Segregation of particles in a square tumbler](image)

The core of steel particles is already almost completely absent of blue glass beads and lobes are already beginning to form due to the mobility of the steel beads relative to glass beads.

The dynamics of particles in a rotating equipment are often unpredictable largely due to the large parameter space. If we consider a simple circular vessel containing two types of particles, there are as many as eight parameters that could govern the behavior of such a system. These can be divided into macroscopic and microscopic parameters. Examples of the macroscopic parameters include the fill level of particles, the vessel size, shape and the rotational speed of the vessel.
Microscopic parameters which may have long term or large scale effects on the evolution of the tumbler are particle size differences, particle density and even surface roughness of the particle.

In a rotating tumbler, there are two macroscopic forces that determine the operation, gravity and centrifugal force. The ratio of these is the Froude number and the regime of operation of the tumbler can be reliably predicted by the Froude number. Six regimes of tumbler operation have been identified\(^{106}\) all of which bear relationship to \(Fr\): the slipping, avalanche, rolling, cascading, cataracting and centrifuging regimes.

We restrict the scope of this work to the rolling regime where the Froude number is, \(10^{-4} < Fr < 10^{-2}\), where gravity dominates over centrifugal force but a continuously flowing active layer of particles exists. We consider only binary mixture of particles. In this regime, the bed of particles is rotated with the tumbler as a fixed bed until a critical point is reached where the angle the free surface makes with the horizontal becomes greater than the angle of repose. At this critical state, the region of particles closest to the surface fails and adjacent layers of particles begin to flow relative to themselves to give a non-zero strain rate.

If specie A is larger than B, and both have the same density, a core of particles containing the smaller particles will be formed. This results from the percolation of smaller particles in the active layer through the pore spaces of the larger particles. The active layer is thickest at the center and smallest at the end because of the zero relative motion of particles to the domain boundaries. The area available for percolation of A relative to B is highest at the center of the active layer and percolation is therefore highest here. This leads to a gradually increasing core of particles centrally located in the vessel. As smaller particles percolate downwards, the larger particles are displaced upwards, get caught in the convective flux of the active layer and swept to the domain boundary.
If the particle differ on the basis of density, we will observe that a tumbler operating in the rolling regime would also have similarities to a system with size differences. Buoyancy will ensure that the particles with higher density would displace lighter particles upwards in the active layer and a radial core of particles would become more well-defined as time progresses.

The situation is more complex when size differences and density differences oppose each other such that particles with a smaller diameter have lower density. The two driving forces for segregation (buoyancy & percolation) oppose themselves. Depending on the ratio of these effects, we can roughly estimate what the equilibrium segregation entropy would be. For example, in a fully segregated system at equilibrium, the segregation intensity would be highest. However, as we alter the density or size ratio or both, we can reduce the equilibrium segregation value. If we correctly select the density and size ratios, we can completely eliminate segregation for a given equipment.

If the domain is thin enough as to eliminate axial segregation but large enough to reduce end wall effects, we progressively begin to see a clear radial segregation of particles with the smaller ones at the core and the larger at the periphery. It is worth mentioning that if you had a long tumbler, axial segregation might also be observed with alternating bands of large and small particles. This axial segregation is due to the difference in repose angle of the two particles. While interesting, axial segregation is not of interest to us in this present paper.

5.5 Validation

In order to validate the computational method used, we make qualitative and quantitative comparisons of the evolution of the segregation intensity for square-shaped tumblers to experimental observation. The dynamical evolution of a given bi-disperse system is similar for
either a circular or square tumbler as it follows both a mechanism of percolation of smaller, denser particles into the core adjacent to the active layer and the buoyancy of larger, lighter particles that have a relative upward flux in the active layer and are conveyed to the periphery of the tumbler.

Based on an equivalent diameter of the tumbler, the Froude number, \( Fr = 0.018 \) which falls within the range of rolling operation for the tumbler \(^{106}\). Tumbler dimensions are 0.25 by 0.25 by 0.0064m\(^3\). Two types of particles are present in an “S+D” type mixture where the effects of Size and Density complement one another. The Size ratio is 0.5 while the density ratio of the larger particles to the smaller particles is 3.0. The drum is half filled with a total of \(~140,000\) particles with both species of particles having the same volume. The bed exists in an initially well mixed state. In order to generate the initially mixed state, the computational particles are initially well spaced and the radius of the glass particles is increased gradually with time in order to avoid large overlaps with the other particles. Once the desired particle size is reached, the growth of the particles stops, gravity is turned on and the simulation begins. Gravitational acceleration is \( g = 9.81 \text{m/s}^2 \). Other parameters for the simulation are given in table 5-1.

Table 5-1: Parameters used in the validation of the DEM code

<table>
<thead>
<tr>
<th>Particle 1</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Density</td>
<td>2520kgm(^3)</td>
<td></td>
</tr>
<tr>
<td>Diameter</td>
<td>2mm</td>
<td></td>
</tr>
<tr>
<td>Number of particles</td>
<td>15,200</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Particle 2</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Density</td>
<td>7500kgm(^3)</td>
<td></td>
</tr>
<tr>
<td>Diameter</td>
<td>1mm</td>
<td></td>
</tr>
<tr>
<td>Number of particles</td>
<td>106,576</td>
<td></td>
</tr>
</tbody>
</table>

| Normal Restitution Coefficient | 0.95 |
| Friction Coefficient          | 0.4  |
| Young’s Modulus               | 2.0E8 Pa |
| Poisson Ratio                 | 0.25  |
Figure 5-6 shows qualitative results of streaking behavior as similar to figure 5 of square tumbler at 50% fill of Jain, Ottino and Lueptow. The pattern is formed in as few as 5 revolutions.

![Figure 5-6: Segregation and streaking of a mixture of steel particles (red, 1mm) and glass beads (blue, 2mm) in a square tumbler comparison to Jain, Ottino and Lueptow](image)

The lobed core that is typical of granular systems with a fill level of 50% is observed. As the flow progresses, smaller, heavier steel particles descend to the core of the bed but because of the extra fluidity, they push towards the domain constraints of the vessel. The longest physical constraint for the flow of particles is at the corners of the domain hence the core stretches into both corners occupied by the bed. This provides explanation to the two-lobed structure.

In order to provide quantitative comparison to experiments, we adopt the measure of segregation similar to that presented in Jain, Ottino and Lueptow where the basis of the index is the area covered by each species of particle as seen from the front view of the mixing device. A mixing/segregation index based on the volume of material in the device might be difficult to extract.
from experiments real-time without altering the granular flow pattern. The area-based segregation intensity is given by equation 5.1:

\[ I = \frac{\left[ A \left( \frac{L^2}{2} - A \right) \right]^{1/2}}{L^2/2} \]  

(5.1)

We validate our simulation against 3 cases with a bi-disperse distribution of particles within a square domain rotating with an angular velocity of 0.21 rad/s\(^{-1}\) Jain, Ottino and Lueptow\(^9\)\(^2\). Glass and steel are the materials used. In all cases the bed is initially well-mixed. The domain dimensions are 0.25 by 0.25 m\(^2\) in cross-sectional area and 3.2 times the diameter of the larger particles. Case 1 is a so-called “D” system of particles containing both steel and glass beads where the size of the particles is 4mm and the driving force for segregation is the particle density only. The evolution of the intensity of segregation for this case is shown in figure 5-7, A.

![Figure 5-7: Time evolution area-based segregation intensity for simulation(red line with star) and experiments Jain, Ottino and Lueptow\(^9\)\(^2\)(blue cross): (A) “D” system with 4mm steel balls and 4mm glass balls; (B) “S+D” system with 3mm steel balls and 4mm glass balls; (C) “S+D” system with 1mm steel balls and 2mm glass balls;](image)

109
De-mixing is predicted by our simulations after 1 revolution and the steady state value of the segregation index matches well with what is obtained by the experiments. Case 2 is an “S+D” system where buoyancy and percolation simultaneously drive the radial segregation of the system. The larger particles (glass balls) have the smaller density. The ratio of particle sizes is 3:4 while the density ratio remains 1:3. Figure 5-7, B shows the evolution of segregation intensity for case 2 and indicates that de-mixing is achieved also around 1 revolution of the tumbler. The steady state value is also predicted by our DEM simulations but in comparison to dynamics of the uniform size mixture, there is more oscillation around the steady state value. We will attempt to draw a relationship between the oscillation of the segregation index and the constantly changing surface length in subsequent sections. Case 3 is a more adverse form of Case 2 in the sense that the particle size ratio for the glass to the steel particles is 2:1. Figure 5-7, C shows the evolution of the segregation intensity and shows that the de-mixing process is even more rapid than the previous two cases. Complete segregation is achieved in 0.7 revolutions and the extent of segregation as seen by the steady state value is closer to the maximum possible value than for the previous cases. The oscillatory behavior towards the end indicates the mass motion of streaks that result from the mobility of the central core of small but dense steel particles.

5.6 Mixing quantification

While the measure of mixing presented in the previous section for validating our simulation approach has good experimental utility because of the simplicity of performing image analysis, its usefulness is limited in quantifying the state of the bed especially when the system can no longer be described as quasi-2D and the core of the bed is difficult to decipher from mere observations at the ends of the vessel. It is important therefore to use a quantification of mixing that conserves the microscopic information of the bed for analysis of the bed dynamics.
5.6.1 Entropy of mixing

Traditional measures of quantifying mixing really on the variance of some local property over the entire domain\textsuperscript{107, 108}. The number density of particles of a given specie is such a property. This is a reliable measure of segregation or mixing when the sample cell size is 1.) Significantly larger than the particle size and 2.) The individual particle species are of the same size. Using the variance of the volume fraction as a local property presents a more reliable means than a mixing index based on number density as we can represent the probability of a given specie using its volume fraction. This comes with a caveat that we have a scheme for accurately determining the volume fractions of each species in a given computational cell. There has appeared in the literature a method that accounts for the volume occupied by a particle that is partially housed by a host computational cell\textsuperscript{23}. The method is fully analytic and can accurately calculate the volume fraction even for structured and unstructured finite volume type sample cells. Calculating mixing indexes either through a number density or a volume fraction based approach suffer from the similar deficiency that they are highly dependent on the length scale of observation. There isn’t a lot of clarity as to what the scale of observation\textsuperscript{109}. At high enough length scales, a mixture of particles in a vessel may be described as well mixed, whereas if we go to lower length scales and study mixing, the same system can be declared segregated. It might be important to define the sampling length scale while comparing it to the macro-length scale of the system in order to have a good idea of mixing characteristics in the vessel of interest.

Doucet, Bertrand and Chaouki\textsuperscript{110} mention that measures of mixing should satisfy 4 criteria, frame invariance, connection to spatial coordinates, property connection and sample size invariance. A proper measure of the mixing index should also provide lower and upper bounds in a non-arbitrary fashion. They define a mixing index based on the correlation of the particle
trajectories to the initial condition. In other words, it is assumed that the mixed state is the equilibrium state of such a system.

5.6.2 Concept of non-equilibrium entropy in granular systems

If we consider a mixture of two sets of particles with a tendency to segregate, either an “S”-system, a “D”-system or an “S+D” –system where both size and density differences drive the flow from a mixed state to a segregated state, we can describe our knowledge of the system in terms of the probability distribution, \( p \), that would be related to the volume fraction of each species in our binary system. For example, let us define \( p \) as a micro-scale ratio of particles in contact with a test particle of species \( A \) indistinguishable from the test particle to the total number of particles in contact with the test particle – figure 5-8 shows an illustration of this picture with the smaller red particles representing species \( A \) (steel balls) and the blue particles representing glass beads. The test particle is \( A^* \) which is indistinguishable from other species \( A \) particles. Thus, the microscopic coordination number fraction can be expressed as equations (5.2a) and (5.2b) that accounts for particles of a given species in contact with the test particle. This definition of coordination number fraction is borrowed from particle number fractions of Chandratilleke, Yu, Bridgwater and Shinozaka \(^{111}\) but normalized by the radius of the particle in contact since we will be considering a bi-disperse system.

\[
p = \frac{(C_{n,A} + 1) r_A^3}{(C_{n,A} + 1) r_A^3 + C_{n,B} r_B^3} \quad \text{(5.2a)}
\]

\[
p = \frac{C_{n,B} r_B^3}{(C_{n,A} + 1) r_A^3 + C_{n,B} r_B^3} \quad \text{(5.2b)}
\]
The addition of 1 in the numerator and denominator accounts for the test particle itself. If we aggregate the coordination number fraction as given by equation (5.2), we would have as many as $N_p$ number of discrete local states of the system where $N_p$ is the total number of particles. In order to determine the entropy, we will then have to perform and ensemble of all the discrete states as defined by $p$ over the entire system. The entropy for $N_p$ equally likely states will be given by

$$S^*\left(N_p\right) = k \cdot \log N_p$$

(5.3)

Where $k$ is analogous to the Boltzmann constant for gases and is a function of the average translational velocity of particles and the granular temperature. If we rewrite as $S^*\left(N_p\right) = -k \cdot \log \left(\frac{1}{N_p}\right) = -k \cdot \left\langle \log p_i \right\rangle$, we can get a good estimation for the entropy. Furthermore, let us add that the ensemble average can be defined as a weighted sum of the probabilities of the various local states of the system where the weights would be the discrete probabilities, we get an expression for $S\left(N_p\right)$ as:
Where \( j \) is a counter for the particles and \( k \) is absorbed into \( S^* \) to give an expression for the informational entropy. There are a few characteristics this property has: first, if the “\( p \)”s are all equal, meaning that all the particles in the granular system see the same coordination number fractions in a regular or close to regular lattice arrangement, \( S \) assumes its highest value. In a binary system, that will correspond to the particles being homogeneously mixed; second, addition of local states that have a probability of zero does nothing to skew the ensemble average as \( \lim_{p \to 0} p \log p = 0 \), hence, the entropy is robust to isolated pockets of unmixed granular material;

One other benefit of using microscopic coordination number based entropy of mixing is that your sample size is truly macro-scale invariant. Regardless of how large, or small the system is, even when the scale is of the order of the particle size, the reliability is preserved.

In order to normalize the entropy, we can define a maximum possible mixing entropy as one that corresponds to the best possible homogeneous system given the overall fractions of each type species in the system. If we define the overall fraction of the individual species with respect to the overall number of particles in the granular bed, we obtain:

\[
P_l,\text{global} = \frac{N_l \cdot r_i^3}{\sum_{i=1}^{N_{\text{species}}} N_i \cdot r_i^3}
\]  

\( N_l \) is the number of particles of specie \( i \) in the entire mixture. In theory, microscopically speaking, the most homogenously mixed state would occur when each particle is in contact with other particles in the mixture in a way that preserves the global volume fraction in equation (5.5)
Hence, summing the entropy over all particles in the bed we obtain equation 5.6 where the global volume fractions are used to construct the most ideal mixed state

\[
S_{\text{max}} = -N_{\text{total}} \cdot \sum_{i=1}^{N_{\text{species}}} p_{i,\text{global}} \ln p_{i,\text{global}}
\]  

(5.6)

It is easily observed that the minimum value for the entropy, \(S_{\text{min}}\) is zero.

### 5.7 Flow in irregular shaped tumbler

We perform numerous simulations to quantify the de-mixing process of an initially well-mixed system of particles in different shaped tumblers and at different fill levels. Analysis is made of the mixing characteristics in 6 different shaped tumblers. These are shown in figure 5-9.

![Figure 5-9: Various computation domains used in the simulations](image)

The first three are based on a circular shape with three different aspect ratios, \(\gamma\) (\(\gamma = 1.00\) corresponding to a circular cross-section and subsequently referred to as tumbler e0; \(\gamma = 1.56\), corresponding to an elliptical cross-section and subsequently referred to as tumbler e1; and \(\gamma = 2.25\) corresponding to an even more eccentric tumbler and subsequently referred to as tumbler e2). The aspect ratio is defined as the ratio of the length in the major dimension (x) to the length in the minor dimension (y). Likewise, the second set of tumblers are based on a rectangular cross-section
with the same set of aspect ratios as the elliptical tumblers ($\gamma = 1.00$ corresponding to a square and subsequently referred to as tumbler r0; $\gamma = 1.56$, a rectangular cross-section and subsequently referred to as tumbler r1; and $\gamma = 2.25$, a more eccentric rectangular shaped tumbler and subsequently referred to as tumbler r2;). For all 6 domains, a mixture of the two species of particles in equal proportions by volume is seeded to $\frac{1}{4}$ and $\frac{1}{2}$ of the volume of the tumbler. The rotation speed of the tumblers is set to 0.42rads$^{-1}$ (corresponding to Fr = 0.0085) which falls within the rolling regime ($10^{-4} < Fr < 10^{-2}$). The direction of rotation is in the positive z direction using a right-hand corkscrew convention. At this value of Fr, gravitational forces dominate over centrifugal forces and the interfaces of the bed remains roughly flat with an angle of repose related to the coefficient of friction between the particles and the walls. Figure 5-10 shows the profiles of the particles in the various computational domains and configurations after 20revs. The particles are initially randomly distributed.

Figure 5-10: Particle distribution after 20 revs in various shaped tumblers. The first row is for an elliptical tumblers at $\frac{1}{2}$ fill while second row is for rectangular tumblers at $\frac{1}{2}$ fill. The displacement of the core of particles towards the left is due to the direct
5.7.1 Particle trajectory

The advantage of using computational studies to investigate granular flow lies in the ability to extract detailed information about the flow field. Figure 5-11 shows the velocity field for a well-developed rotating drum for a rotation cycle. Each velocity field is obtained from an axial slice at the center of the bed. In each phase of the cycle, there is a noticeable flowing layer where the bed is sufficiently dilated and adjacent particle layers are in relative motion with each other.

The bulk of the bed however is inactive with respect to a non-inertial frame of reference moving with the rotation velocity of the tumbler. This is as a result of the non-zero weight of the over-burden on inner regions within the bed and the high frictional force at the walls. As a result of the well-defined flow-field of particles in a perfectly circular tumbler, the particle trajectories are expected to be steady with minor drifts from the streamlines. We focus on the particle

Figure 5-11: Velocity Field of a circular tumbler at ¼ fill
trajectories in the x-y plane and try to explain the differences in the motion of particles in a circular vessel as opposed to vessels with irregular shape. Figure 5-12, A shows the motion of two particles in tumbler e0 – glass (red path-lines) and steel (blue path-lines). Both particles start at the filled circle and terminate at the star. Figure 5-12, B shows the accompanying segregation after a few revolutions of the circular tumbler.

![Fig 5-12](image)

Figure 5-12: (A) Particle trajectories in circular tumbler for small steel particles (red) and large glass beads (blue) (B) Radial segregation in tumbler.

Because of the perfect rotational symmetry of the tumbler, the particles follow an orbital path as a result of the fixed bed, reach the surface and translate from the top end of the surface to the bottom end. Due to buoyancy differences, the large (but less dense) particles end up on the periphery of the bed while the smaller (more dense) particles spiral into the center of the radial core of particles. Despite the preferential path of the particles shown, random stream line crossings are not common in this regime of tumbler operation for this vessel. This is because of the relatively constant flow layer length. One consequence of the nature of this type of flow is the concentricity in the segregated region of particles that a circular tumbler attains.
If we however use elliptical tumbler e1 with a non-circular cross-section, the particle trajectories become altered. Figure 5-13 show the path of the smaller steel particles. In order to facilitate comparison, the scales of the particle trajectory figures are all the same. We decide not to superimpose the two trajectories in the interest of clarity. The chaotic nature of the particle trajectory by merely changing the ratio of the major and minor tumbler axis is clear. The motion of steel particles as shown in figure 5-13 is comprised of multiple “whirls” that result from the exit and re-entry of particles into a constantly changing flow layer. The flow layer is longest when the angle of repose is aligned parallel to the major axis of the elliptical vessel and lowest when aligned parallel to the minor axis of the vessel.

![Figure 5-13: Particle Trajectory in tumbler e2 with an aspect ratio equal to 2.25](image)

The effect of disturbing the rotational symmetry and thus altering the streamlines of particles in the tumbler has been described by Christov, Ottino and Lueptow who called it “streamline jumping”. We will show in subsequent sections that the whirling motion of particles has consequences of introducing harmonic frequencies on top of the fundamental frequency of
rotation of the vessel as dictated by the angular rotation speed when the long term time dependent mixing entropies are analyzed. It also helps in enhancing the rate and extent of segregation.

5.7.2 Effect of aspect ratio on segregation dynamics

Figure 5-14 shows a comparison of the dynamics of segregation in tumblers e0 (red lines), e1 (blue lines) and e2 (pink lines). We show the coordination-based entropy of mixing as defined earlier to quantify the process of segregation. This entropy is normalized by the maximum value for the mixing entropy as illustrated in equation 5-6.

![Figure 5-14: Evolution of mixing entropy for various tumblers](image)

(A) For tumblers e0, e1 and e2 at ¼ fill, (B) For tumblers e0, e1 and e2 at ½ fill

In all cases, the particle bed starts from a well-mixed state and rotation is started impulsively at time 0. In all cases the number of particles is roughly the same for a given fill level (about 16,000 for the ¼ fill, 32,000 for the ½ fill). The ratio of the total volume of large particles to small particles is roughly 1:1. Figure 5-14 shows that segregation the dynamics of segregation proceed asymptotically from a mixed to a de-mixed state for all three circular based geometries at a fill level of ¼. In addition, we see that the dynamics of tumbler e2 are fastest albeit with an
oscillatory nature. The development of entropy for tumbler e1 is less rapid with a lower amplitude at its steady state. Except for a small amount of noise, tumbler e0 shows no gross oscillatory patterns and a much slower segregation dynamic. The story is much the same for ½ filled vessels. The deviation of the shape of the vessel from the base circular cross-section gives rise to gross oscillations in the motion of the segregated core of particles and consequently the enhancement of the rate of segregation. It should also be noted that if we compare the corresponding curves on figure 5-14, A to those of 5-14, B, we observe slower dynamics when a higher fill level of particles is tumbled. The drop of the rate of segregation as a function of fill level is a well-reported phenomenon\textsuperscript{100,113} that is due to the development of dead zones that do not cycle through the active flowing layer at the top of the bed.

Figure 5-15: Evolution of mixing entropy for various tumblers (A) For tumblers r0, r1 and r2 at ¼ fill, (B) For tumblers r0, r1 and r2 at ½ fill,

Likewise, figure 5-15 shows the segregation in rectangular tumblers. In figure 5-15, A we see that the segregation process proceeds to a greater extent as we go from a square to a rectangular vessel. And just as we saw earlier for elliptical vessels, the dynamics for ½ filled rectangular vessels is slower than the corresponding ¼ filled vessels as evidenced by figure 5-15, B. In all
cases, there is observed fluctuation of the entropy of mixing with the square having the least fluctuations while the rectangular geometry with the largest aspect ratio having the largest fluctuations.

5.7.3 Spectral analysis

Mobility of the central core of steel particles relative to the glass particles on the periphery is a source of an added dimension of chaos as we will see in a power spectrum analysis of the steady state entropy values. This may help to explain why an elliptical tumbler enhances the process of segregation. As the core of particles stretch and contract with the surface of the bed, a faster rate of expulsion of larger particles from that core into the flowing layer results. In figure 5-16 we perform a Fourier analysis of the entropy of mixing time series for tumbler e2 at ½ fill. Our sample time frequency is an integer multiple (100 times) the frequency of rotation (rotation speed is 0.42rads-1).

It should also be observed from the Fourier analysis that the magnitude of the amplitude is strongly dependent on the aspect ratio of the tumbler. Take for instance figure 5-18, A and C which show the frequency spectrum at ¼ fill for tumblers e1 and e2 respectively. We see that the magnitude of the component for the fundamental frequency (recall that for this section, rotation speed of the tumbler is \( \omega = 0.42 \text{rads}^{-1} \), corresponding to \( f_0=0.133 \text{Hz} \)) is lower for tumbler e1 (aspect ratio, \( \gamma = 1.56 \)) than it is for tumbler e2 (aspect ratio, \( \gamma = 2.25 \)). Also the higher harmonics are not distinguishable in figure 5-16, A. The argument is quite the same for the ½ filled tumblers as shown in figures 5-16, B and 5-16, D. The reason why we now observe the higher harmonics in figure 5-16, B than in 5-16, A is because of the larger number of particles in this case. Likewise, the higher harmonics register more noticeable signals in figure 5-16D than in 5-16C because of the larger number of particles used in extracting the mixing entropy.
Figure 5-16: Frequency spectrum in (A) tumbler e1 at ¼ fill, (B) tumbler e1 at ½ fill, (C) tumbler e2 at ¼ fill, (D) tumbler e2 at ½ fill.

The largest peak is the one corresponding to twice the speed of rotation at 0.133Hz. This is because of the mirror symmetry of the vessel around each major axis, hence a half rotation can be seen as corresponding to one cycle. As the tumbler rotates, the stretching and contraction of the interface occurs twice each revolution thus accounting for the oscillatory particle dynamics in the core of the bed. In addition to the fundamental frequency, two other peaks of decreasing magnitude are observed at exactly, 0.266Hz and 0.399Hz as seen in figures 5-16, B, C and D. These are exact harmonics of the base frequency (i.e. $2f_0$ and $3f_0$) This is perhaps due to the fact that in addition to the stretching and contraction mechanisms of the elliptical tumbler, the relative fluidity of the core of steel particles may result in faster replenishment of unsegregated particles to the active layer at the top of the bed. Figure 5-17 shows the motion of the centroid of the core of particles in tumbler e1.
This process drives the segregation of particles at a faster rate than if the mobility of the core were eliminated in a circular based tumbler. In figure 5-17 we show the motion of the center of gravity of the dense, smaller steel balls for ½ filled tumbler e1. The drift of the quickly formed core of particles tracked by this center of gravity may resemble an attractor in x-y space. The center of gravity starts out in a cyclical series of orbits on the left of figure 5-17 (beginning at the filled circle) and gradually drifts to a more stable orbit on the right (terminating at the star). The direction of rotation of the vessel is clockwise.

Figure 5-17: Motion of the centroid of the core of steel particles beginning at the filled circle and terminating at the star.

We plot the frequency spectrum for the Fourier analysis of the rectangular tumblers in figure 5-18. Figure 5-18, A and B are for tumbler r1 (aspect ratio, $\gamma = 1.5$) at ¼ and ½ fill respectively while figures 5-18, C and 5-18, D are for tumbler r2 (aspect ratio, $\gamma = 2.25$) at ¼ and ½ fill respectively. As noted for the elliptical tumblers, the primary frequency is seen at 0.133Hz, again corresponding to the two instances when the surface of the bed is stretched to its longest
extent during each cycle of the tumbler rotation. Figure 5-18 A shows harmonics at $2f_0$. Figure 5-18, C in comparison to 5-18, A shows that at the same fill level, if we increase the aspect ratio of the tumbler, we can excite the third harmonic frequency ($3f_0$). While the energy present in the fundamental frequency in figures 5-18, B and 5-18, D are clearly larger than 5-18, A and C respectively, it is not entirely clear why higher harmonics are not considerably excited.

![Frequency spectrum in (A) tumbler r1 at ¼ fill, (B) tumbler r1 at ½ fill, (C) tumbler r2 at ¼ fill, (D) tumbler r2 at ½ fill](image)

5.8 Conclusion

In this work we have explored the enhancement of the dynamics of segregation in irregular shaped rotating tumblers by examining elliptical and rectangular tumblers operating in the rolling regime. We define a new entropy of mixing that relies on the local coordination information of each particle and its size to construct a truly sample-size invariant entropy of mixing for dense
granular systems. We have shown that the cause for improved dynamics as compared to that of a circular tumblers is due to the stretching and contraction of the active layer of the tumblers which shows up as higher order harmonics when a spectral analysis is performed on the entropy of mixing time series.
Chapter 6 Summary

In conclusion, we present a summary of the major contributions of this work.

6.1 Application of DEM-CFD to study particle cluster sedimentation

We were able to show that the discrete element method coupled with computational fluid dynamics can reproduce some of the interesting features associated with the settling of a cluster of particles in an ambient viscous liquid. These features include particle leakage, torus formation, breakup and dispersion. We validated the settling of a swarm of particles against available literature and show that in comparison to simple point source methods, a volume averaged momentum formulation and a Lagrangian particle approach can give better agreement with the experiment. This is especially true as the volume exclusion effect becomes more pronounced as seen in high volume fraction dispersions.

We applied the same procedure to studying the interaction between 2 clusters of particles and quantify the structural changes in the evolution of the swarm of particles are fundamentally different depending on how where we initialize the cluster of particles. We also show similarity that particle clusters bear with drops of fluid in an immiscible ambient.

6.2 Development of new drag law for gas-solid fluidization

We showed that the application of existing drag laws to modelling fluidization behavior in a gas-solid fluidization may be inadequate. An over prediction of pressure drop and velocity profiles is obtained using popular closure laws. This is primarily due to the origin of these closure laws being rooted in uniform liquid-solid fluidization. We made an attempt to address this problem by performing an energy balance across a fluidized bed to account for the production of inhomogeneous flow structures in bubbles and slugs. We are able to show better performance than
existing drag laws in not only attenuating the pressure drop but also the transverse velocity profile for a small-scale fluidized bed.

6.3 Application of DEM-CFD to show that increased chaos in rotating drums as a result of irregular drum geometry leads to accelerated segregation dynamics

We applied the discrete element method to simulating the behavior of a binary system of two spherical particles with different size and densities to predict segregation. We validated our method against available data in the literature. We developed a new method of quantifying segregation and use it to study segregation in various tumbler shapes and show that an acceleration of segregation dynamics will result when the shape of the tumbler is more prolate. Hence, an elliptical tumbler with a high aspect ratio –major axis divided by minor axis – will show a greater acceleration of the segregation process as opposed to low aspect ratio elliptical tumblers.
References

5. S. Ergun, Chemical Engineering Progress 48, 89-94 (1952).


23. C. Wu, J. Zhan, Y. Li, K. Lam and A. Berrouk, Chemical Engineering Science 64 (6), 1260-1266 (2009).


43. B. Metzger and J. E. Butler, Phys Fluids 24 (2) (2012).


69. R. H. Wilhelm and M. Kwauk, Chemical Engineering Progress 44 (3), 201-218 (1948).


Appendix A: Analytical Solution for the Settling Velocity of a Swarm of Particles at Low Reynolds Number

If we briefly revisit the origin of equation 3.6: if we begin from the assumption that a collection of particles can approximate the behavior of a drop of liquid settling in an immiscible ambient, the Hadamard-Rybczynski equation can be applied to describe its settling speed. Therefore:

\[ V_c = \frac{2 R^2 g (\rho_c - \rho)}{3} \frac{\mu + \mu_c}{\mu (2\mu + 3\mu_c)} \quad (A1) \]

The density of the suspension drop is \( \rho_c \). The viscosity of the suspension drop, \( \mu_c \), can be related to the viscosity of the ambient fluid by Einstein’s equation through the volume fraction:

\[ \mu_c = \mu (1 + 2.5\phi) \quad (A2) \]

If we substitute for \( \mu_c \) in equation (A1) we get

\[ V_c = \frac{2 R^2 g (\rho_c - \rho)}{3} \frac{\mu}{\mu} f(\phi) \quad (A3) \]

Where \( f(\phi) = \frac{2+2.5\phi}{5+7.5\phi} \)

If we linearize \( f(\phi) \),

\[ f(\phi) = \frac{4 - \phi}{10} + O(\phi^2) \quad (A4) \]

Substitute back in (23) and noting that \( \rho_c - \rho = \phi(\rho_p - \rho) \)
\[ V_c = \frac{4}{15} \phi \frac{R^2 g (\rho_p - \rho)}{\mu} - \frac{1}{15} \phi^2 \frac{R^2 g (\rho_p - \rho)}{\mu} + O(\phi^2) \]  

Divide through by the terminal settling velocity: \( u_0 = \frac{2(\rho_p - \rho)a^2 g}{9\mu} \), noting \( \epsilon = \frac{a}{R} \) and \( \phi = N\epsilon^3 \) and neglecting higher order terms,

\[ v_c^* = \frac{V_c}{u_0} = \frac{6}{5} N\epsilon - \frac{3}{10} N^2 \epsilon^4 \]

As done by Nitsche and Batchelor \(^1\), the essential point of this approximate derivation is to show that the slope of the relation between \( v_c^* \) and \( N\epsilon \) is 1.2. Since the connection between Hadamard-Rybczynski’s fluid-fluid analysis and the effective suspension concept is only approximate, it is not expected to be valid over a broad range of \( N \) and \( \epsilon \). We assert that if we have a reasonably large number of particles, our simulation approach should capture the factor \( K(=1.2) \) in the equation.
Appendix B: Derivation of New Drag Law for Simulation of Gas-Solid Fluidization

B1: Pressure drop in expanded beds

In order to derive the drag on each particle in an expanded bed we borrow from arguments for pressure drop in fluidized beds as expressed in 78 and 67.

B1.1: Laminar contribution to coefficient of drag

The analysis begins with the expression of pressure drop in a straight tube as given by the Hagen-Poiseuille equation in the laminar regime

\[ \Delta P = \frac{32\mu V_L L}{D_e^2} \]  \hspace{1cm} (B1)

Where \( D_e \) is the equivalent diameter given in equation (B2).

\[ D_e = 4 \times \frac{\text{cross-sectional area for the flow}}{\text{wetted perimeter}} \]  \hspace{1cm} (B2)

\[ = 4r_H \]

\( V_L \) is the velocity of the continuous phase, \( \mu \) is the viscosity, \( L \) is the length of the bed of particles.

If we note that the axial pressure drop balances the shear stress at the walls we can get a definition for the hydraulic radius. The Hydraulic radius comes from

\[ \Delta P A_T = \tau_s S \]  \hspace{1cm} (B3)
\( S \) is the surface area available to flow, \( A_T \) is the cross-sectional area available to flow and \( \tau_s \) is the shear stress at the surface available to flow. Therefore,

\[
\tau_s = \frac{\Delta P V}{L S} = \frac{\Delta P}{L} r_H 
\]

(\text{B4})

\( r_H \) is the hydraulic radius. By definition, we can relate the hydraulic radius to the cross-sectional area available to the flow when the tube contains particles and the surface area exposed to the fluid by all particles in the system. Equation (B5) is a mathematical expression of this.

\[
r_H = \frac{\pi}{4} \frac{D^2 \varepsilon_G}{\pi \varepsilon \frac{d_p^3}{6}} = \frac{\varepsilon_G}{6 \varepsilon_S} d_p
\]

(\text{B5})

\[
D_e = \frac{4 \varepsilon_G}{6 \varepsilon_S} d_p
\]

(\text{B6})

If we substitute into the pressure drop equation,

\[
\Delta P = \frac{72 \mu V_G L \varepsilon_S^2}{d_p^2 \varepsilon_G^3}
\]

(\text{B7})

This pressure drop accounts for only skin friction hence correction has to be made for form drag.

There are two approaches in correcting for form drag,

1. By modeling the form drag as a function of the volume fraction of solids since this value directly affects the tortuosity of the bed.
Hence an expression for the total pressure drop is given:

\[ \Delta P_T = \Delta P_S + \Delta P_F \]  

(88)

\( \Delta P_F \) is the form drag while \( \Delta P_S \) is the skin drag as given by equation (B7). The form drag is due to the tortuosity hence is related to the volume fraction of the solid particles and the total pressure as:

\[ \Delta P_F = \varepsilon_s \Delta P_T \]  

(89)

\( \Delta P_T \) is the total pressure drop

Substituting into expression for skin drag

\[ \Delta P_T = \frac{72 \mu V_G L \varepsilon_s^2}{d_p^2 \varepsilon_g^3} \]  

(10)

In the case of a fixed bed where \( \varepsilon_L = 0.4 \),

\[ \Delta P_T = \frac{180 \mu V_G L \varepsilon_s^2}{d_p^2 \varepsilon_g^3} \]  

(11)

2. By modifying the hydraulic radius of the bed

If we define the pressure drop as contributed to by skin drag and form drag we can write

\[ \tau_F + \tau_s = \frac{\Delta PV}{L S} \]  

(12)

Or

\[ \tau_s = \frac{\Delta P}{L S} \frac{V}{1 + \frac{\tau_F}{\tau_s}} \]  

(13)

\( \tau_F \) is a stress attributable to form drag. Hence, hydraulic radius is:
\[ r_H = \frac{V}{S \left( 1 + \frac{\tau_F}{\tau_S} \right)} \]  

(B14)

Bird, Stewart and Lightfoot \(^{114}\) show that \( \frac{\tau_F}{\tau_S} = 0.5 \) when the particle Re is in the laminar regime

Thus

\[ r_H = \frac{\varepsilon_G}{\varepsilon_S} d_p \]  

(B15)

\[ D_e = \frac{4 \varepsilon_G}{\varepsilon_S} d_p \]

Substituting into Hagen-Poiseuille (equation B1) and replacing \( V_G \) by the true velocity \( V_L/\varepsilon_L \),

\[ \Delta P = \frac{162 \mu V_G L \varepsilon_S^2}{d_p^5 \varepsilon_S^3} \]  

(B16)

We can recast for applicability to non-fixed beds (where \( \varepsilon_L \neq 0.4 \))

\[ \Delta P = \frac{64.8 \mu V_G L \varepsilon_S^2}{d_p^5 \varepsilon_S^4} \]  

(B17)

This equation doesn’t reduce to a form consistent with the Stokes settling velocity when \( \varepsilon_L \to 1 \) and should be modified accordingly.

For a bed containing \( N \) particles, if we correlate the volume of a single particle to the drag force around the particle, the force balance for the bed is \( \frac{\pi D^2}{4} \Delta P = \frac{\pi D^2 L \varepsilon_S}{v_p F_D} \) and \( v_p \) is the volume of a single particle.

\[ \frac{\Delta P}{L \varepsilon_S} = F_D \]  

(B18)

Substituting for the pressure drop from equation (B16)
From Stokes equation, for a single particle the drag force is:

\[ F_D = 3\pi \mu d_p V_G \]  

(B20)

Therefore the drag force seen by a single particle when we combine the effects of neighboring particles with the drag in an infinite medium in the creeping flow regime the force on a single particle becomes

\[ \frac{\Delta P v_p}{L \epsilon_s} = \frac{10.8\pi d_p V_G \mu \epsilon_s}{\epsilon_G^4} \]  

(B19)

\[ \frac{\Delta P v_p}{L \epsilon_s} = 3\pi \mu d_p V_G \left[ \frac{3.6\epsilon_s}{\epsilon_G^4} + 1 \right] \]  

(B21)

If we note that the coefficient of drag is \( C_D \), where

\[ C_D = 6 \frac{\epsilon_G^{-4.8}}{Re_p} \]  

(B23)

It is often the case that the bracketed portion of equation B23 is represented in power law format such that

\[ C_D = 6 \frac{\epsilon_G^{-4.8}}{Re_p} \]  

(B24)
Assumptions are that form friction is proportional to the projected area of particles and the shear drag is twice the form drag. Figure B-1 shows us a collapse between the laminar portion of the Ergun equation and a Wen & Yu type volume fraction dependence.

At equilibrium, the drag force is balanced by the net force between gravity and buoyancy, therefore

\[ F_D = 3\pi \mu d_p V_{s\infty} = \left( \rho_p - \rho \right) \frac{\pi d_p^3}{6} g \quad \text{(B25)} \]

Where \( V_{s\infty} \) is the slip velocity in an infinite medium. Therefore, equating to earlier expression for \( F_D \) since force balance on rhs is independent of volume fraction we can relate \( V_{s\infty} \) to \( V_L \),

\[ \frac{V_G}{V_{s\infty}} = \left[ \frac{3.6 \varepsilon_s}{\varepsilon_G^4} + 1 \right]^{-1} \approx \varepsilon_G^{4.8} \quad \text{(B26)} \]
B2.1.2: Turbulent contribution to the coefficient of drag

According to the drift-flux law, the slip velocity is given by equation (B27)

\[ V_{slip} = \frac{V_G}{\varepsilon_G} \pm \frac{V_s}{\varepsilon_s} \]  \hspace{1cm} (B27)

The energy input rate for fluid input into a bed at minimum fluidization is

\[ E_i = AV_{G1} g H_1 (\varepsilon_{s1} \rho_s + \varepsilon_{G1} \rho) + A(V_{G2} - V_{G1}) g H_2 (\varepsilon_{s2} \rho_s + \varepsilon_{G2} \rho) \]  \hspace{1cm} (B28)

\( \varepsilon_{s1} \) is the solids fraction without bubbles; \( \varepsilon_{G1} \) is the gas fraction without bubbles; \( V_{G1} \) is the inlet velocity without bubbles; \( H_1 \) is the height of the bed less head attributable to the bubbles; \( \varepsilon_{s2} \) is the average solids fraction with bubbles; \( \varepsilon_{G2} \) is the gas fraction with bubbles; \( V_{G2} \) is the inlet velocity above the minimum bubbling velocity; \( H_2 \) is the height of the bed including the head attributable to the bubbles.

Fluid leaving the bed has an energy of

\[ E_l = AV_{G1} g H_1 \rho + A(H_2 - H_1)(V_{G2} - V_{G1}) \rho g \]  \hspace{1cm} (B29)

The first term on the rhs of equation (B29) is the energy in the fluid leaving a bed that is purely homogeneous (say at incipient fluidization) while the second term on the rhs of equation (B30) is the additional head due to the presence of bubbles. The net power dissipation in the bed is given by a balance between the energy input rate and the energy leaving at the top of the bed.

\[ E_B = E_i - E_l \]  \hspace{1cm} (B30)

\[ E_B = A g (\rho_s - \rho)[V_{G1} H_1 \varepsilon_{s1} + (V_{G2} - V_{G1})(H_2 - H_1) \varepsilon_{s2}] \]  \hspace{1cm} (B31)
By performing a force balance on a particle on the basis of surface area, we have equation (B32)

\[ C_d \pi d_p^2 \frac{1}{2} \rho V_{G2}^2 = \frac{\pi}{6} d_p^3 (\rho_s - \rho) g \] (B32)

Substituting for the density difference in equation (B32) using equation (B31) and using the necessary mathematical manipulations,

\[ E_B = \frac{3AH_2 \varepsilon_{s2} C_d \rho V_{G2}^3 K}{d_p} \] (B33)

\( K \) is given by \( \left[ \frac{V_{G1}}{V_{G2}} + \left( 1 - \frac{V_{G1}}{V_{G2}} \right) \left( 1 - \frac{H_1}{H_2} \right) \right] \). If we replace \( V_{G1}, H_1 \) and \( \varepsilon_{s1} \) by the values at minimum fluidization velocity, \( V_{G,mf}, H_{mf} \) and \( \varepsilon_{s,mf} \) and we drop the 2 in the subscript for actual gas flow rate and noting that since the cross-sectional area of the bed is constant, the Height of the bed has an inverse proportional relationship with the average solid volume fraction, i.e. \( \frac{H_1}{H_2} = \frac{\varepsilon_{s2}}{\varepsilon_{s1}} \) we get equation (B35)

\[ E_B = \frac{3AH \varepsilon_s C_d \rho V_G^3 K}{d_p} \] (B34)

\( K \) is hence \( \left[ \frac{V_{Gmf}}{V_G} + \left( 1 - \frac{V_{Gmf}}{V_G} \right) \left( 1 - \frac{\varepsilon_s}{\varepsilon_{s,mf}} \right) \right] \). The energy dissipation per unit mass of gas in the bulk of the bed, \( E_m \) can be obtained by dividing equation (B35) by \( \varepsilon_G H A \rho \)

\[ E_m = \frac{3AH \varepsilon_s \varepsilon_G C_d \rho V_G^3 K}{d_p \varepsilon_G} \] (B35)

The cube root of the product of the power dissipation per unit mass of the fluid and turbulent intensity should be of the same magnitude as the velocity fluctuations, \( U' \) in the bed.
\[ U' = (E_m I)^{1/3} \]  

(B36)

By analogy to the friction factor in a straight pipe, the coefficient of drag is related to the radial component of the fluctuating velocity through equation (B37)

\[ C_D' = 2 \left( \frac{U'_r}{V_G} \right)^2 \]  

(B37)

We assume that the turbulent intensity is twice the diameter, \( I = 2d_p \), of the particle and that the radial component of fluctuating velocity is half the velocity fluctuations, \( U'_r = U'/2 \) and substituting for \( E_m \) in equation B35 we obtain:

\[ C_D' = 2 \left( 1.5 \frac{\varepsilon_s K}{\varepsilon} \right)^2 \]  

(B38)

In a dynamic bed, the overall fluid turbulence is contributed to by the bulk turbulence and the form turbulence hence,

\[ \left( \frac{U}{V_{slip}} \right)^2 = 1.5\varepsilon_s + \left( \frac{U_{\infty}}{V_{slip}} \right)^2 \]  

(B39)

The first term on the RHS is from the bulk turbulence intensity due to presence of other particles while the second term is from the form turbulence intensity. This will apply at inlet velocities when particles begin to fluctuate or larger.

It is known that the mean square fluctuation velocity in the axial direction is 2.5 times higher than in the axial direction,

\[ U_z = 2.5U_x = 2.5U_y \]  

(B40)

Hence if \( U^2 = U_x^2 + U_y^2 + U_z^2 \), \( U_z = 0.87U \)
From the force balances the net between buoyancy and gravity gives the drag hence we can have a relationship between \( C_D \) and \( C_D' \) under equilibrium conditions

\[
\frac{V_{\text{slip}}}{V_{\text{slip,}\infty}} = \left( \frac{C_D'}{C_D} \right)^{1/2}
\] (B41)

Substituting for the expressions for coefficient of drag,

\[
\frac{V_G}{V_{\text{slip,}\infty}} = \varepsilon_G \left( \frac{C_D'}{C_D + C_D'} \right)^{1/2} = \varepsilon_G \left( \frac{1}{C_D'/C_D' + 1} \right)^{1/2}
\] (B42)

\( C_D' = 0.11 \) and using the expression derived for \( C_D' \)

\[
\frac{V_G}{V_{\infty}} = \varepsilon_G \left( \frac{1}{40.91\varepsilon_S^2 K^2 + 1} \right)^{1/2}
\] (B43)

It can clearly be seen that

\[
C_D = C_D' (40.91\varepsilon_S^2 K^2 + \varepsilon_L^2)\varepsilon_L^{-2}
\] (B44)

In the limiting case where \( K = 1 \), the drag coefficient can be approximated as

\[
C_D = C_D' \varepsilon_G^{-4.8}
\] (B45)
Equation (B44) can be combined with the laminar regime drag, equation (B23) or (B24) to get a generalized form for the transition regime noting that for the turbulent regime, $C_{D\infty} = 0.11$ on the basis of surface area of the particle.

$$C_D = \frac{6}{Re_p} \left[ \frac{3.6\varepsilon_s}{\varepsilon_G^4} + 1 \right] + 0.11 \left[ \frac{40.91\varepsilon_s^2 K^2}{\varepsilon_G^2} + 1 \right]$$

(B46)
Appendix C : Letters of Permission

Figure 3-2: Three regimes of cloud settling based on particle and cloud scale inertia is reproduced with permission from material published in Pignatel, F., M. Nicolas, et al. (2011). "A falling cloud of particles at a small but finite Reynolds number." Journal of Fluid Mechanics 671: 34-51. The scanned letter of approval is given:
Chapter 5, a discrete element study of granular segregation in circular and none circular rotating drums, has appeared previously in one of our publications. The publishers have granted us permission for reuse:
Vita

Oladapo Ayeni was born in Lagos, Nigeria, to Oladapo and Modupeola Ayeni. After graduating from secondary school at King’s College, Lagos in 2000, he went on to study Chemical Engineering at the University of Lagos, Akoka, Lagos, Nigeria, earning a Bachelor of Science degree in 2006. Oladapo has some experience working in the financial industry having worked at Zenithbank Plc, Nigeria between September 2008 and December 2009. His decision to retrace his steps back to engineering brought him to pursue a Doctor of Philosophy at Louisiana State University.

Oladapo enjoys observing society, reading and playing soccer in his spare time.