A Study of Particle-laden Flows from Meso and Micro-scale Perspectives

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A STUDY OF PARTICLE-LADEN FLOWS FROM MESO AND MICRO-SCALE PERSPECTIVES

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 in Philosophy in The Gordon A. and Mary Cain Department of Chemical Engineering

by

Daniel Guedes de Oliveira
B.S., Federal University of Ceara, 2014
May 2020
Acknowledgements

First and foremost, I would like to thank God. "...Wisdom and power are his... He gives wisdom to the wise and knowledge to the discerning." - Daniel 2:20-21.

I would like to thank my advisor, Prof. Krishnaswamy Nandakumar, for his support of and enthusiasm about my research and career. He has opened many doors for my professional and personal growth. I would like to express my deepest gratitude to Dr. Chunliang Wu, Prof. Anthony Wachs, Dr. Can Selçuk, Prof. J. B. Joshi, Prof. Peter Minev and Dr. Johnwill Keating, who have contributed directly or indirectly to the completion of this work, for sharing resources, time, critiques and experience with me. I would also like to recognize the members of my committee: Dr. Celalettin Ozdemir, Dr. Karsten Thompson and Dr. Manas Gartia.

I wish to acknowledge past and present members of the EPIC research group: Dr. Rupesh Reddy, Dr. Yuehao Li, Dr. Gongqiang He, Dr. Chenguang Zhang, Dr. Abhijit Rao, Dr. Mutharasu Chockalingam, Dr. Shivkumar Bale, Dr. Mayur Sathe, Dr. Jielin, Dr. Zhizhong Ding and fellow graduate students Sai Ganesan, Sharareh Heidarian and Aaron Harrington, and pay my special regards to Dr. Oladapo Ayeni, who introduced me to CFD-DEM.

I am indebted to friends who helped me persevere in this journey: Can Selçuk, Renato Coutinho, Swarom Kanitkar, Cameron Young, Vikram Gowrishankar and Shashank Tiwari.

I wish to acknowledge the support and great love of my parents and relatives, Silvana Guedes, Denilson de Freitas, Guilherme de Oliveira, Aristarco and Marina Coelho, Jose and Aldenice Paes-Leme and Alvinice de Oliveira. They have provided a solid foundation for my life. I would like to pay homage to my grandfather, Alvimir de Oliveira, who passed away in 2018. Certainly, I have been able to reach this far because of him. Also, I would like to celebrate my son, Andre de Oliveira, born in 2019. His smile brightens my days.

Finally, I dedicate this work to my wife, Lídia de Oliveira, who have been my greatest support and partner in all moments of life.
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Abstract

Particle-laden flows are investigated numerically from a meso-scale perspective using Computational Fluid Dynamics coupled with Discrete Element Method (CFD-DEM) and from a micro-scale perspective using Particle Resolved Direct Numerical Simulation (PR-DNS). For the former, the dynamics of a pseudo-2D pulsed fluidized bed (PFB) consisting of 400,000 to 800,000 particles was investigated (Chapters 2 and 3). The focus is on the capabilities of CFD-DEM to (1) reproduce pattern formation in these systems and (2) further the understanding of the dynamics of PFB’s as a function of pulsation parameters. In Chapter 4, a two-spheres system is investigated with a recently implemented PR-DNS code, using the Basilisk open source framework. A high-resolution study is performed to investigate the flow field structures and their relation to experienced hydrodynamic forces by the spheres under the influence of a wall. In Appendix A, some verification and validation cases are reported with both the aforementioned codes, presenting capabilities that can be further explored in future work.
Chapter 1. General Introduction

1.1 Particle-laden Flows

Flow of matter occurs frequently as a mixture of phases rather than a single phase in isolation. In particular, two-phase fluid-solid systems are present in a variety of environmental and industrial settings, such as oceans, dunes, and atmosphere through the transport of sediments [4]; and in the pharmaceutical, food, mining, and petroleum industries in the form of drying and conveying of powder, ore separation and sand transport in the wellbore. The effective behavior of particle-laden flows can be profoundly different from their single-phase counterparts. For this reason, design, scale-up and optimization procedures for the operations embodying these processes are heavily dependent on a thorough understanding of the intra- and interphase interactions occurring in such systems. Such interactions add to the complexity of single-phase flows by enlarging the spectrum of time and length scales associated with the relevant transport phenomena. Let us take the example of a fluidized bed. At the particle length scale, fluctuations of particles arising from collisions and fluid-particle momentum exchange momentarily create local particle-rich and particle-lean regions – clusters and voids. These local heterogeneities in the system are prone to growth due to the nonlinear dependence of the fluid-solid interaction with the void volume fraction [21, 22] and the dissipative nature of particle collisions [23]. This leads to flow structures of length scales comparable to the size of the equipment enveloping the process. These large structures ultimately affect the averaged quantities of relevance to practical applications, such as the pressure drop and reaction conversion. This shows the intricate connection between phenomena occurring at the micro and macro-scales. This complexity precludes the use of a single overarching numerical methodology to describe these systems. For this reason, it is customary to use a multi-scale modeling approach to investigate such problems, where fundamental, highly-resolved studies sit at the base of a hierarchy of modeling approaches, feeding information into higher levels through closure models [23].
1.2 Numerical Approaches

In this study, particle-laden flows are investigated from meso and micro-scale perspectives, using the following approaches, respectively: (1) computational fluid dynamics with discrete element method (CFD-DEM) and (2) particle-resolved direct numerical simulation (PR-DNS). The two-fluid model approach (TFM) is briefly discussed, since part of its formulation is also used in CFD-DEM.

TFM is a meso/macro scale approach in which both particles and fluid are treated as continua, and field variables, such as volume fraction, pressure and velocity describe the evolution of the phases in an Eulerian fashion. The same time and length scales (computational cell) are used to resolve the fluid and solid flow structures, clusters and voids. The equations describing each phase are derived from a volume-averaging procedure applied to the equations of motion of particles and the momentum and continuity equations of the fluid. The averaging of the solid phase equations cause the details of the particle-particle interactions to be lumped into an effective stress tensor term, while the fluid-particle interactions are accounted for through an averaged interphase momentum exchange term. Both terms need closure; the former one is particularly cumbersome due to the obscurity in the rheology of the granular media and is most frequently described by the kinetic theory of granular gas [25, 26]. The volume-averaged continuity and the fluid-phase momentum equations, which are of relevance to this work, are:

\[
\frac{\partial}{\partial t} (\epsilon \rho_f) + \nabla \cdot (\epsilon \rho_f \mathbf{u}_f) = 0 \tag{1.1}
\]

\[
\frac{\partial}{\partial t} (\epsilon \rho_f \mathbf{u}_f) + \nabla \cdot (\epsilon \rho_f \mathbf{u}_f \mathbf{u}_f) = -\epsilon \nabla p + \nabla \cdot (\epsilon \mathbf{\tau}) + \mathbf{S}_f + \epsilon \rho_f \mathbf{g} \tag{1.2}
\]

with the viscous stress tensor evaluated as: \( \mathbf{\tau} = \mu (\nabla \mathbf{u}_f + \nabla \mathbf{u}_f^T) + \frac{2}{3} \mu (\nabla \cdot \mathbf{u}_f) \mathbf{I} \). The following variables \( \epsilon, \rho_f, \mu, \mathbf{u}_f, p, \mathbf{g} \) and \( \mathbf{S}_f \) stand for void fraction; fluid density, viscosity, velocity and pressure; acceleration of gravity; and the interphase momentum source-sink term. These equations are adopted in the CFD-DEM modeling framework for the the fluid phase. However, the evolution and contact dynamics of the solid phase is performed.
at a relatively high resolution, where each particle is tracked via Newton’s second law of
motion and the kinematic equation. The governing equations for the translational and
rotational motion of a particle $i$ with mass, $m_{p,i}$, and volume, $V_{p,i}$ are as follows:

$$m_{p,i} \frac{d{u_{p,i}}}{dt} = F_{f-s}^{p,i} + \sum_j (F_{cn,ij} + F_{ct,ij}) + m_{p,i}g \quad (1.3)$$

$$I_i \frac{d{\omega_{p,i}}}{dt} = \sum_j (R_i n_{ij} \times F_{ct,ij}) + T_{f-s}^{p,i} + T_{\text{rolling}} \quad (1.4)$$

$$\frac{d{x_{p,i}}}{dt} = {u_{p,i}} \quad (1.5)$$

The motion of particles are driven by fluid-solid hydrodynamic interactions, $F_{f-s}^{p,i}$ and
$T_{f-s}^{p,i}$, body forces such as gravity, and collisional interactions with other $j$ particles, $F_{cn,ij}$,
$F_{ct,ij}$ and $T_{\text{rolling}}$. The latter term is the torque resistance arising from the rolling motion
of particles. The total fluid hydrodynamic force, $F_{f-s}^{p,i}$, arising from the relative motion
of fluid and particles can be divided into three components: (1) a term from pressure
contribution, modeled as $V_{p,i} \nabla p$; (2) the drag force, which acts in the direction of the slip
velocity $u_f - u_p$; and (2) the lift force, which acts in the tangent plane with respect to the
drag force. The contribution to the drag force may be further divided into: steady-state
drag, added mass effect, and Basset force. The latter two effects appear when considering
the transient motion of a particle and are associated to accelerating the surrounding fluid
and the lagging development of the boundary layer, respectively. Among the different
terms composing the drag force, the steady-state drag component dominates over the
transient and non-uniformity terms, particularly in gas-solid systems, since these terms
are inversely proportional to particle to fluid density ratio [11]. For this reason and be-
cause of the difficulties in the implementation of other terms, the steady-drag has received
most attention when it comes to the development of drag force correlations [12-14]. Lift
force arises as a result of particle rotation and wake asymmetry effects. Depending on the
source of rotation, the lift force can be identified as the Saffman force or Magnus force.
The first is associated with a rotation induced by a fluid field velocity gradient, while the
second can have any source for rotation such as particle collisions [11]. Recently, new correlations were produced for the lift force based on direct numerical simulations [15]. However, these forces have been mostly neglected when modeling industrial applications, as the magnitude of lift forces are considerably smaller than drag forces and because correct prediction of averaged quantities, such as pressure drop, can be obtained using only the steady-state drag models [16]. Nevertheless, these forces may play a significant effect in environmental flows, suspending sediments at the bottom of the ocean as a result of both gradients and collisions as well as in industrial applications, such as pneumatic conveying. In this work, the steady-state drag is modeled by the Gidaspow correlation in the CFD-DEM approach [29]:

\[
\beta = \begin{cases} 
150(1 - \epsilon)^{2}\mu + 1.75(1 - \epsilon)^{2}d_{p}^{2}p\|u_{r} - u_{p}\|, & \text{if } \epsilon \leq 0.8 \\
(3/4)C_{D}\epsilon(1-\epsilon)\rho f|u_{r} - u_{p}|\epsilon^{-2.65}, & \text{if } \epsilon > 0.8
\end{cases}
\] (1.6)

where \(C_D\) is the drag coefficient for a single particle:

\[
C_D = \begin{cases} 
\frac{24}{Re_{p}} (1 + 0.15Re_{p}^{0.687}) & \text{if } Re_{p} \leq 1000 \\
0.44 & \text{if } Re_{p} > 1000 
\end{cases}, \quad Re_{p} = \frac{\epsilon d_{p}^{2}}{\mu} |u_{r} - u_{p}|
\] (1.7)

The following equations show how the drag force on a single particle and the source-sink term are modeled:

\[
F_{d} = \frac{V_{p}}{1-\epsilon} \beta (u_{r} - u_{p})
\] (1.8)

\[
S_{f} = -\frac{1}{V_{cell}} \int_{V_{cell}} \sum_{k=1}^{N_{p}} F_{d,k} \delta(x - x_{p,k})dV
\] (1.9)

where \(V_{cell}\) and \(F_{d,k}\) are respectively the mesh cell volume and the drag force acting on particle \(k\). Regarding the collision dynamics, there are three relative motions when particles contact each other: sliding, rolling and spinning. The first motion is associated with the relative linear velocity of the particles at the contact point; whereas the other two are associated with the relative angular velocity in the tangential and normal direction at
the contact point, respectively. Each of these motions give rise to resisting forces, which in turn affect the energy dissipation and post-collision motion of particles. The contact forces and moments are calculated based on the distribution of stresses over the contact area, which forms as particles deform [17]. However, the full description of the collision phenomenon is too expensive for computational purposes and hence simple mechanical models are used to obtain the contact forces [18]. Cundall and Strack [19] introduced mechanical elements—dashpot, spring and slider—to describe the normal \( F_{cn} \) and tangential \( F_{ct} \) components of the contact force. The normal and tangential forces are characterized by a spring stiffness \( k \), damping coefficient \( \eta \), and friction coefficient \( \mu \), and each force contains two terms—elastic and dissipative:

\[
F_{cn} = -\left( k_n \delta_n + \eta_n u_n \right)
\]

\[
F_{ct} = -\left( k_t \delta_t + \eta_t u_t \right)
\]

The variables \( \delta \) and \( u \) stand for particle overlap and relative velocity at the contact point. Sliding between contacting particles is described by Coulomb’s law of friction, \( |F_{ct}| > \mu |F_{cn}| \), and once in the dynamic friction regime the magnitude of the tangential force is given by \( \mu |F_{cn}| \). With the exception of the friction coefficient, which may be obtained empirically, the other parameters \( (k, \eta) \) are chosen in a manner as to match characteristic aspects of collision, such as collision time and coefficient of restitution as well as reversal of tangential velocity in oblique contacts [18, 20]. In addition, dynamic characteristics of damped oscillators may be used to estimate the damping coefficient. This description of collision allows the particles to overlap slightly. This is the so-called soft-sphere approach, where the true deformation of particles are described by this virtual overlap and the collision process is tracked.

Contact mechanics also provides fundamental insights into how these terms may be evaluated. The two most commonly used theories are the Hertzian theory for elastic and frictionless spheres and Mindlin’s theory of frictional spheres. The former introduces a nonlinear spring to normal collisions: \( k_n \delta_n^{3/2} \), where \( k_n = 4/3 \sqrt{R_{eff} E_{eff}} \) can be evaluated.
through physical properties of the particle material, such as the Poisson ratio ($\nu$) and the Young’s modulus ($E$). An estimate of the collision time is also given by this nonlinear spring, which is inversely proportional to $k_n^{2/5}$. The latter theory relates the tangential displacement with the tangential force through $k_t = (2\sqrt{2R_{eff}}G)/(2 - \nu)(\delta_n^{1/2})$, which is also based on particle material, such as the Shear modulus, $G$. Tsuji et al. [11] incorporated the Hertz-Mindlin nonlinear contact scheme, for the collision of the particles in a CFD simulation, and proposed a relationship for $\eta_n = \alpha\sqrt{m_{eff}k_n\delta_n^{1/4}}$, such that the dissipation of energy after a collision is only a function of the restitution coefficient which is incorporated through the $\alpha$ factor. They also assumed $\eta_t = \eta_n$. The CFD-DEM studies presented in this work follows the implementation given in [11]. The CFD side is carried out by the commercial solver Fluent [5], while the DEM side was developed by Dr. Wu, a former postdoctoral researcher at Louisiana State University. The DEM code is written in user-defined functions that are coupled to the CFD solver.

The micro-scale approach consists in resolving all the relevant time and length scales of the problem. In systems where turbulence is not significant, particles impose these minute scales, and the term particle-resolved direct numerical simulations has been coined to describe this approach [27]. Because the flow around particles are resolved, fluid-particle interactions are calculated directly from velocity and pressure fields; while particle motion is described in a Lagrangian fashion. The classical continuity and Navier-Stokes equations for incompressible flows are used:

$$\nabla \cdot \mathbf{u}_f = 0 \quad (1.12)$$

$$\frac{\partial}{\partial t}(\rho_f\mathbf{u}_f) + \nabla \cdot (\rho_f\mathbf{u}_f\mathbf{u}_f) = \nabla \cdot \mathbf{\sigma} + \rho_f\mathbf{g} \quad (1.13)$$

and Newton’s equation of motion and kinematic condition for each particle:

$$m_{p,i}\frac{d\mathbf{u}_{p,i}}{dt} = \int \mathbf{\sigma} \cdot \mathbf{n} dS + m_{p,i}\mathbf{g} \quad (1.14)$$

$$I_{p,i}\frac{d\omega_{p,i}}{dt} = \int (\mathbf{x} - \mathbf{x}_{p,i}) \times (\mathbf{\sigma} \cdot \mathbf{n}) dS \quad (1.15)$$
Here the forces considered in Equations (8), (9), and (10) are only due to external forces. Note that the hydrodynamic forces are directly computed from the total stress tensor, \( \sigma = -pI + \mu(\nabla u_f + \nabla u_f^T) \). Many approaches have been developed to solve these equations in domains of time-dependent complex shape associated with multiphase flows. Two general approaches of discretization of the equations can be defined: conforming and non-conforming. In conforming approaches, the domain is continuously re-meshed so that the shape of the dispersed phase can be accommodated. These are high accuracy approaches that demand a significant amount of computational resources due to continuous re-meshing of time-dependent domains. On the other hand, non-conforming approaches extend the mesh over a larger, simpler domain which includes both fluid and dispersed phase. For this reason, they are also called fictitious domain methodologies. Accuracy is compromised by not resolving boundaries precisely, although the gain in speed is substantial. The variation of this latter approach is mainly due to how equation and boundary conditions are implemented on the dispersed phase [29]. The code used in this study is a combination of three parts: Basilisk + DLM/FD + Grains3D. Basilisk is an open source partial differential equation solver developed on a adaptive Cartesian mesh framework. The other two components have been implemented and coupled to Basilisk by Dr. Wachs and Dr. Selcuk at University of British Columbia, Canada. The DLM/FD stands for the Distributed Lagrange Multiplier based Fictitious Domain method. It has been first proposed and implemented to solve particle-laden flows by Glowinski et al. (1999) [30]. Grains3D is a DEM module developed by Dr. Wachs [97]. More details about the solvers used here are given in the next chapters.

1.3 Outline

Two problems were chosen for the detailed investigation of their physics with the numerical approaches mentioned previously: (1) the dynamics of pulsed fluidized beds and (2) wall-induced hydrodynamics.

Oscillation of the inflow to a fluidized bed has long been utilized as a mechanism for enhanced fluidization quality. In 2003, Coppens and Ommen revealed another aspect of this mode of fluidization by introducing a sinusoidally oscillated flowrate \( V = V_M + \)
$V_A \sin(2\pi ft)$, to a pseudo 2D bed of particles. Regular patterns of bubbles emerged from the distributor as opposed to the chaotic formation found in continuously fluidized systems. This was reported as a means of gaining more control over the fluidized bed by the addition of two more degrees of freedom, frequency and amplitude of oscillation.

In this work, we investigate the effect of the mean flow velocity term, $V_M$, and the amplitude of oscillation, $V_A$. A preliminary study was carried out to determine whether our models contain the minimum physics for producing staggered patterns, which is shown in Chapter 2. Quantitative effects of the variation of pulsation parameters, $V_M$ and $V_A$, are investigated in Chapter 3.

Particle-laden flows near a stationary wall are extremely relevant for a variety of problems. The applications range from microfluidics devices to large scale sediment transport in oceans. Although, the effect of stationary walls to multiple-particle systems have been investigated before, a detail analysis of the effect of walls on the hydrodynamic interactions between particles is still lacking. In Chapter 4, wall-induced hydrodynamics are investigated considering two spheres in tandem arrangement.

Finally, in Chapter 5, the contributions of these studies are summarized and possible future works are described, referencing incipient investigations presented in Appendix A.

2.1 Introduction

Fluidization is one of the most prominent operations in industry and many developments have followed since its first commercial use, demonstrating its versatility in enhancing the intimate contact between phases. However, as a multiphase system, there are enormous challenges in its theoretical, experimental and computational analysis. The modelling of multiphase flows in industrial equipment is often based on empiricism. In order to promote advancement in optimization and scale-up activities, there needs to be fundamental understanding of the underlying mechanisms of this operation and its derivatives.

The oscillation of gas inflow to fluidized bed is a technique used for promoting the fluidization quality through reduction of by-passing and channeling [102]. Pulsed fluidized beds (PFB) have been categorized on the basis of how the pulsation is implemented. Operations which produce pulsation through oscillation of the flow stream are classified as intermittent; whereas operations which acquire pulsation by alternating the flow to different sections of the bed are classified as relocating gas stream systems [38]. Many advantages associated to the use of this technique have been reported. Zhang and Koksal (2006) experimentally studied the effects of intermittent oscillation of flow on heat transfer and obtained improvements up to three times of that found in steady flow systems. Applying an alternating pattern of intermittent and steady flow, Akhavan et al. (2009) were able to reduce agglomeration of particles, thus enhancing drying procedures and fluidization quality. Furthermore, relocating implementations of PFB were developed for the pulp and paper sludge drying process [51]. Newer methods for operating pulsed fluidized beds are constantly being developed [27].

Of note is the work by Coppens et al. (2003) who found regular, periodic patterns when the input gas flowrate is oscillated. They implemented pulsation through the superposition of a constant stream of gas with an oscillating component while maintaining the

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bed always above minimum fluidization condition. The experiments were carried out in quasi-two-dimensional beds for sand-air system. When the gas flow was oscillated, rows of bubbles were generated such as to form hexagonal patterns with each row staggered with respect to the previous one. There are three important remarks made by Coppens et al. about this phenomenon: (1) The structured arrangement of bubbles is not a result of linear resonance since there is a range of frequencies for which the phenomenon occurs; (2) the bed width is a crucial parameter to the stability of the pattern; the wider the bed, the more persistent the bubble pattern; and (3) the inter-bubble distance is independent of frequency and width within the range of frequency and size that allow the realization of the pattern. Wang and Rhodes (2005) performed a 2D DEM study of this phenomenon. They raised important questions as to the stability of the patterns with respect to the pulsation parameters - frequency, amplitude and wave format – providing answers based on pressure analysis and snapshots of the bed. The bubble patterns do not appear to be as regular as those observed in the experiments by Coppens et al. They attributed this to the fact that the thickness of the bed simulated by 2D DEM (one particle diameter) was much smaller than the one used by Coppens et al. The formation of what they called “horizontal channel-like” (HC) structure was given as a necessary condition for the organized structure formation. The present work intends to provide new insight into the underlying mechanisms of ordered flow structures in pulsed fluidized bed following the three experimental assertions made by Coppens et al. (2003) and making connections between observations and the literature on bubble formation and dynamics. A 3D discrete particle modelling approach is used for all simulations. The objective of this work is to reproduce the patterns reported experimentally and to assess its sensitivity with respect to particle size and pulsation parameters.

2.2 Problem Description

A 3D bed of rectangular cross section was used in the simulations. The dimensions together with particle and fluid properties are specified in Table 2.1. The contact scheme parameters are also presented. The bed was given no-slip boundary conditions for its lateral walls, and a zero gauge pressure for the outlet. The inlet velocity contains a
constant term superimposed by an oscillatory term as described by Coppens et al.

Table 2.1. Parameters used in the CFD-DEM simulations.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Particle diameter ($d_p$)</td>
<td>420 - 550 µm</td>
</tr>
<tr>
<td>Particle density ($ρ_p$)</td>
<td>2650 kg/m³</td>
</tr>
<tr>
<td>Restitution coefficient ($e$)</td>
<td>0.95</td>
</tr>
<tr>
<td>Poisson ratio ($ν$)</td>
<td>0.25</td>
</tr>
<tr>
<td>Coulomb friction coefficient ($μ_C$)</td>
<td>0.2</td>
</tr>
<tr>
<td>Young’s modulus ($E$)</td>
<td>$2 \cdot 10^8$ Pa</td>
</tr>
<tr>
<td>Fluid density ($ρ_f$)</td>
<td>1.225 kg/m³</td>
</tr>
<tr>
<td>Fluid viscosity ($μ$)</td>
<td>$1.8 \cdot 10^{-5}$ Pa · s</td>
</tr>
<tr>
<td>Bed ($W \times H \times T$)</td>
<td>16 x 32 x 0.2 cm³</td>
</tr>
</tbody>
</table>

$$V = V_M + V_A \sin(2πft) \quad (2.1)$$

where $V_M$ is the constant velocity term; and $V_A$ is the amplitude of the oscillatory velocity.

Equation 2.1 is scaled by the minimum fluidization velocity.

Coppens et al. (2003) used Geldart B particles and reported a range of values for which bubble patterns were formed: $V_M = 1.2 - 1.7$; $V_A = 0.2 - 0.7$; and $f = 2.5 - 7$ Hz. Table 2.2 shows the parametric space investigated in this work, which was chosen so as to reflect the experimental conditions. More details of the numerical schemes and models may be found in Chapter 1 and Chapter 3.

Table 2.2. Pulsation parameters.

<table>
<thead>
<tr>
<th>Set</th>
<th>Particle diameter</th>
<th>Particle density</th>
<th>Frequency</th>
<th>$V_M$</th>
<th>$V_A$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>550, 550, 420</td>
<td>2650</td>
<td>3.5</td>
<td>1.3</td>
<td>0.3</td>
</tr>
<tr>
<td>2</td>
<td>420</td>
<td>2650</td>
<td>3.5</td>
<td>1.4, 1.3, 1.2, 1.1</td>
<td>0.4, 0.3, 0.2, 0.1</td>
</tr>
<tr>
<td>3</td>
<td>420</td>
<td>2650</td>
<td>2, 3.5, 5</td>
<td>1.3</td>
<td>0.3</td>
</tr>
</tbody>
</table>

2.3 Results and Discussion

Set 1 in Table 1.2 gathers the simulations carried out for the purpose of studying the effect of particle size on bubble patterns. Figure 2.1 presents the void structures generated over a time span of 2 times the period of oscillation. Regular patterns were observed for the 420 µm particles case, which produced a 1-2-1 type of bubble pattern persistent in time. From the simulations, it is noticeable that rows generated for smaller particles grow into staggered bubbles more frequently than that for larger particles. Higher degree of
Figure 2.1. From top to bottom: 550, 500, 420 $\mu m$ particle systems with $f = 3.5 \text{ Hz}$, $V_M = 1.3$, $V_A = 0.3$.

Figure 2.2. From top to bottom: $V_M/V_A = 1.4/0.4$, $1.3/0.3$, and $1.1/0.1$ with $f = 3.5 \text{ Hz}$ and $d_p = 420 \mu m$.

organization was perceived with the decrease of particle size for the parameters used in set 1.

Set 2 shows the computational experiments where the effect of $V_M$ and $V_A$ was studied. The constant component and the amplitude of the oscillating component were both simultaneously changed by 0.1 from one simulation to the other. As the parameters were reduced, bubble size also decreased, and another recognizable pattern was evidenced for the case where $V_M/V_A = 1.4/0.4$, which presented a zig-zag pattern, as shown in Figure 2.2. The bubble pattern lost its strength as $V_M/V_A$ was changed to $1.2/0.2$, and subsequently to $1.1/0.1$. Although, in the very beginning of these cases patterns emerged and repeated over 3 periods of oscillation.
Figure 2.3. From top to bottom: $f = 2.0; 3.5; \text{ and } 5.0$ with $V_M = 1.3, V_A = 0.3, \text{ and } d_p = 420 \, \mu m$.

The frequency effect was investigated by evaluating frequencies of 1.5 Hz apart from the $f = 3.5$ Hz case, which was already shown to produce patterns for the conditions. As shown in Figure 2.3, the higher frequency case produced smaller bubbles. Although bubbles in different rows were staggered, regular patterns were not observed due to coalescence and break-up of bubbles. For the lower frequency case, the distance between rows increased significantly, resulting in low interaction between rows through the bubbles’ hydrodynamics. The variation of inter-bubble distance with frequency is not experimentally observed as stated in assertion 3. However, both of the cases mentioned did not produce regular bubble structures. It may be the case that the smaller bed width restricted the range of frequencies for which bubble patterns are stable, but further work is necessary to verify that.

From a frame-by-frame analysis of the simulation results, the HC structure is identified as a precursor of each new row of ordered bubbles, as observed by Wang and Rhodes. This prompted us to evaluate how the structure evolved into the patterns. Figure 2.4 shows the HC structure for the 1-2-1 pattern case. The images indicate that the HC structure is affected by the row ahead of it, which influences the number of bubbles present in the forming row.

As is known, bubbles serve as shortcuts for the gas phase when their velocity is less than the interstitial velocity in the emulsion phase [52]. The hydrodynamics of a
bubble allows the incoming gas, especially below it, to flow through the bed, reducing the accumulation of gas in that particular region of the HC structure. Together with this comprehension, our simulations suggest that the patterns initiate through a cascading process. Once the system has reached the right conditions for the realization of patterns, the number of bubbles in one row will dictate the number and position of bubbles in the following row and so on.

2.4 Conclusion

The objective of this work was to produce regular patterns through pulsation and study the effect of particle and pulsing parameters on them. The CFD-DEM approach was shown to be successful in capturing the regular void structures that arise when pulsation is applied. As particle size was decreased the degree of organization increased for $f = 3.5$, $V_M = 1.3$ and $V_A = 0.3$. Additionally, the number of bubbles forming in the HC structure was shown to be dependent on the number of bubbles in the row ahead of it. For small frequencies, the distance between the HC structure and the row ahead increases, and this interaction does not occur as strongly as for smaller distances. However, as the distance is reduced by an increase in frequency, coalescence of bubbles disturbs the patterns. Further work is needed to fully comprehend the suppression of chaos through pulsation and in consequence bubble patterns.

3.1 Introduction

The enhanced heat and mass transfer capabilities of fluidized beds have been its gateway to a variety of industries. Coal gasification, catalytic cracking, sulfide roasting and olefin polymerization are only a few of the successful applications of this unit. Invigorated interest has emerged due to new and pressing demands such as processing of ultra fine powder - nano-scale size - and clean energy production. The basic implementation of fluidized beds consists of suspending a bed of particles by imposing an upward-moving fluid flow. Fluidization is attained once the flow rate produces a pressure drop equivalent to the net buoyant weight of the particle bed. However, the flow regime at this point and at higher flow rates depends on a number of other factors, such as vessel geometry, type of distributor, particle and fluid properties, operating conditions, etc. The delicate dependence of solid and fluid flow patterns on this large number of variables results in a complex process, whose scale-up and effective operation have historically been performed as individualized and empirical activities with many modifications to address the challenges and to optimize the phenomena occurring inside the fluidized bed [107, 52, 28].

Oscillating the fluid phase flow rate is an example of such modifications that affects both intra- and inter-phase interactions and can lead to improved fluidization quality. Total pulsation systems that implement pulsation by completely shutting off the inflow of fluid are among the most studied cases in the literature. This type of operation is linked to enhancement of heat transfer as well as improvement of fluidization quality in cohesive systems [115, 44, 19]. However, it may also lead to strong defluidization, restricting operating variables (e.g. low frequencies or high mean flow rate) [44] or requiring assistance from other mechanisms, such as vibration [42]. Furthermore, long “off” periods may cause large pressure build-up before the particle bed, making the process irregular [44, 4].

An alternative to this implementation is the partial pulsation system, in which a
primary flow supports the bed under fluidization, while a secondary stream provides os-
cillation [18]. This approach has been shown to yield the enhanced fluidization quality
associated with total pulsation, reducing minimum fluidization velocity in PFB’s contain-
ing nano-particle material and permitting fluidization in the first place for large particle
systems [32, 2, 64, 101, 61]. On the other hand, experimental investigations on drying of
biomass material suggest that this alternative could diminish the effectiveness of pulsation
in breaking up inter-particle forces. This is due to the smoothing of the pressure “shock”
generated in total pulsation systems [44, 42, 41]. Preliminary experimental studies also
indicate that heat transfer improvements associated with total pulsation are either the
same or superior to the ones with partial pulsation unless for specific oscillation frequen-
cies [114]. The choice of which methodology to apply strongly depends on the final goal
of its application. However, in order to promote industrial use of this technology, it is
desirable to design a robust PFB system [38]. With this in mind, further exploration of
the different regimes of pulsation is indispensable.

The impact of pulsation parameters - mean superficial velocity \((V_M)\), amplitude \((V_A)\)
and frequency \((f)\) - have been investigated by both experimental and numerical ap-
proaches, with particular emphasis on the effects of \(f\) [38]. The PFB transitions between
three regimes as \(f\) is increased. At low frequencies, explosive expansions of the particle
bed, followed by counter-current flow of the phases, is observed during the high-velocity
period (also called “on” or active phase). Subsequently, during the low-velocity period (or
“off”, inactive phase), a static bed is formed. This behavior has been described as purely
intermittent. The second regime, observed at intermediate frequencies, is described as a
piston-like fluidization since the bed moves up and down as a macroscopically compacted
system with the periodical formation of void layers at the bottom. Void layers (or slugs)
grow and disintegrate into bubbles that erupt at the surface. Within this intermediate
stage, the increase of \(f\) causes new void layers to emerge while residual void structures
are leaving the bed. As frequency is increased both said periods are reduced, which
causes weaker bed expansion and incomplete settling of particles; thus, inducing a less
intermittent behavior [115, 42, 10, 106, 46]. The third regime is characterized by high
frequencies, above the natural frequency of the system. In this regime, the bed loses its capacity to respond to oscillations and acquires a behavior similar to the one without pulsation, producing smaller bubbles and diminished bed expansion [46, 68, 43, 11].

The effects of the other two parameters, \( V_M \) and \( V_A \), have been less explored, although previous studies have assessed their influence on the PFB through measurements of drying efficiency, surface-to-bed heat transfer coefficients and bubble size. In general, the increase in \( V_M \) produces diminishingly higher surface-to-bed heat transfer coefficients, with optimum values dependent on the imposed frequency [115, 44]. In addition, higher drying rates were obtained with increased values of \( V_M \), which were explained as the result of better gas-solid contact and mixing [41]. At intermediate frequencies (2-4\( Hz \)), both the bubbling intensity and the bubble size have been reported to increase with \( V_M \) [106, 100]. Less information is available regarding the effect of \( V_A \), especially because in total pulsation systems \( V_A \) and \( V_M \) are not independent, since the base flow, \( V_M - V_A \), is fixed and equal to zero. Studies on partial pulsation systems show that as \( V_A \) is increased, a larger amount of gas is introduced into the bed, causing larger bubbles to form and the appearance of void layers from the bottom of the bed[106, 100]. Furthermore, higher drying rates have been reported with the increase in \( V_A \) within intermediate frequencies (2-4\( Hz \)). At such frequencies, the strength of pulsation is reduced, and cohesive interactions between particles hinder effective gas-solid interaction [57].

The relative scarcity of detailed information regarding the effects of \( V_M \) and \( V_A \) together with the necessity of an increased robustness of the PFB technology demands an in-depth exploration of different pulsed flow regimes. Indeed, the increasing demand for renewable energy sources and process intensification highlights the relevance of this work. On one hand, the results obtained here may give new insights for the operation of pulsed fluidized beds used for drying of biomass material [42, 41, 43] and for solar energy storage [39, 86]. On the other, as miniaturization of fluidized beds continue [80, 98, 20, 21], a greater understanding of the effects of pulsation at the micro level will also rise. Motivated by this, the present work aims at understanding the dynamics of the pulsed fluidized bed under the variation of \( V_M \) and \( V_A \) through a computational investigation.
We limit our attention to a pseudo-2D bed composed of Geldart B particles, whose gas inflow velocity is sinusoidally oscillated, \( V = V_{mf}(V_M + V_A \sin(2\pi ft)) \). \( V_M \) assumes three values: 1.1, 1.2 and 1.3. The minimum base, \( V_M - V_A \), and maximum top, \( V_M + V_A \), superficial velocities reach 0.7 and 1.8, respectively. As suggested in previous works [106, 105, 11], such conditions are not the most suitable for the Two-Fluid Model (TFM) approach as frictional particle-particle interactions become more important; thus, making CFD-DEM a more adequate choice for studying these conditions.

3.2 Numerical Methodology

3.2.1 Approach

CFD-DEM is a powerful tool for the simulation of dense particulate systems, especially those with enduring multiple contacts among particles [34]. Its capability in evaluating the PFB behavior is demonstrated by previous works [105, 100, 74]. It is worth mentioning that the detailed results from CFD-DEM simulation in [105] uncovered the mechanisms behind regular formation of bubbles and shed light on the hydrodynamics of PFB’s. In this work, we also adopted CFD-DEM as our simulation tool.

The CFD-DEM approach consists of resolving the fluid flow at the scale of the computational cell, whose size is about one-order larger than the particle size, as in the Two-Fluid Model (TFM) approach; while particle evolution is evaluated from a Lagrangian perspective, tracking each particle through Newton’s equations of motion. This allows a highly resolved description of the solid phase with a relatively cheap implementation when compared to Direct Numerical Simulation approaches.

In this work, we use the well developed in-house parallel code [104] to solve the particle dynamics (DEM). The code is coupled to the CFD solver ANSYS-Fluent [5], which solves the volume-averaged fluid phase equations under finite volume numerical framework. The formulation for these equations correspond to set II in [116], also known as model A. The Euler-implicit time discretization scheme is used, and the pressure-velocity coupling is treated iteratively through the semi-implicit method for pressure-linked equation (SIMPLE). Spatial discretization of the advection and diffusion terms are carried out by the quadratic upwind interpolation of convective kinematics (QUICK)
and central differencing schemes, respectively. Absolute criteria for the convergence of continuity and momentum equations are set to 0.0001. An analytical method is applied for the computation of the void fraction field [103] and an implicit two-phase coupling scheme is used for the integration of the particles equations and source-term evaluation as described in the Chapter 1. The details of such scheme and the parallel implementation of the code can be found in [104].

A soft-sphere approach is used for the collisional dynamics, where the elastic term of the particle-particle interaction is given by the Hertzian-Mindline solid contact description. In addition, the model for the viscous term both in the normal and tangential components of the collisional force follows the implementation suggested in [92]. Sliding between contacting particles occurs once the static friction limit is surpassed. Both static and dynamic friction assume the same value, denoted as the Coulomb friction coefficient.

Table 3.1. Parameters of the CFD-DEM simulations.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Solid phase</strong></td>
<td></td>
</tr>
<tr>
<td>Particle diameter ($d_p$)</td>
<td>420 $\mu$m</td>
</tr>
<tr>
<td>Particle density ($\rho_p$)</td>
<td>2650 kg/m$^3$</td>
</tr>
<tr>
<td>Restitution coefficient ($e$)</td>
<td>0.95</td>
</tr>
<tr>
<td>Poisson ratio ($\nu$)</td>
<td>0.2</td>
</tr>
<tr>
<td>Coulomb friction coefficient ($\mu_C$)</td>
<td>0.2</td>
</tr>
<tr>
<td>Young’s modulus ($E$)</td>
<td>7 MPa</td>
</tr>
<tr>
<td>Minimum fluidization velocity ($V_{mf}$)</td>
<td>0.2 m/s</td>
</tr>
<tr>
<td><strong>Fluid phase</strong></td>
<td></td>
</tr>
<tr>
<td>Fluid density ($\rho_f$)</td>
<td>1.225 kg/m$^3$</td>
</tr>
<tr>
<td>Fluid viscosity ($\mu$)</td>
<td>$1.8 \times 10^5$ Pa·s</td>
</tr>
<tr>
<td><strong>Geometry, Mesh, Time step</strong></td>
<td></td>
</tr>
<tr>
<td>Bed ($W \times H \times T$)</td>
<td>160 x 200 x 2 mm$^3$</td>
</tr>
<tr>
<td>Grid size</td>
<td>2 mm</td>
</tr>
<tr>
<td>Ratio cell to particle volume</td>
<td>206</td>
</tr>
<tr>
<td>Fluid time step</td>
<td>$2 \times 10^{-4}$ s</td>
</tr>
<tr>
<td>DEM time step</td>
<td>$1.0 \times 10^{-5}$ s</td>
</tr>
<tr>
<td><strong>Pulsation parameters</strong></td>
<td></td>
</tr>
<tr>
<td>Mean superficial gas velocity ($V_M$)</td>
<td>1.1; 1.2; 1.3</td>
</tr>
<tr>
<td>Amplitude of oscillation ($V_A$)</td>
<td>0; 0.1; 0.2; 0.3; 0.4; 0.5</td>
</tr>
<tr>
<td>Frequency of oscillation ($f$)</td>
<td>3.5 Hz</td>
</tr>
</tbody>
</table>

Table 3.1 lists the CFD-DEM parameters used to investigate the effect of $V_M$ and $V_A$ on the PFB behavior. The particle bed consisted of approximately 400,000 Geldart B particles, which assumed a settle bed height of 83 mm. Note that $V_M$ and $V_A$ are quantities scaled by the minimum fluidization velocity, $V_{mf}$. The particles were assigned a relatively small Young’s modulus (7 MPa) in order to avoid prohibitively small time
steps. The mesh size (2\text{mm}) was chosen such that adequate computation of void fraction is achieved and meso-scale flow structures are captured. Grid sensitivity is assessed by computing the average particle volume fraction along a line in the middle of the bed (\(y = 40\text{mm}\)) and the power spectrum distribution (PSD) of the particle volume fraction oscillations at (\(x, y\)) = (80, 40)\text{mm} for the case where \(V_M = 1.3\) and \(V_A = 0.5\). Overall the results show little variation with mesh size (Figure 3.1). However, larger deviations occur for the case with fine mesh relative to the other cases: the average volume fraction is slightly lower and the intensity of the dominant peak in the particle volume fraction PSD is significantly higher, although at the same frequency as the others. These differences may be attributed to a higher sensitivity of the particle volume fraction with motion of particles.

The boundary conditions consisted of no-slip at the walls, superficial velocity described by \(V = V_{mf}(V_M + V_A\sin(2\pi ft))\) at the inlet and constant pressure (101325 \text{Pa}) at the outlet. \(V_M\) varied from 1.1 to 1.3, and \(V_A\), from 0 to 0.5. The frequency of oscillation, \(f\), was kept constant at 3.5\text{Hz}, which is the dominant frequency of oscillation one of the cases without pulsation.
3.2.2 Analysis

All the results presented in the next section are collected from the simulated time period between 4 to 8 seconds. This time span is equivalent to 14 full cycles given that the frequency of imposed oscillation is $3.5Hz$. Additionally, statistical and spectral analysis are performed over this range to eliminate the influence of transient effects. The sampling frequencies were 5000 Hz and 50 Hz for pressure and particle volume fraction signals, respectively. The assessment of the particle bed behavior is carried out via the analysis of the following parameters: average coordination number ($CN$), center of mass height (or average height) ($Y_{CM}$) and axial velocity ($V_{CM,y}$), axial bubble granular temperature ($\Theta_{yy}$), pressure signals and particle volume fraction field ($\phi$). Table 3.2 shows how some of these are calculated.

Table 3.2. Parameters used for the analysis of the fluidized beds.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Equations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Average coordination number ($CN$)</td>
<td>$CN = \frac{2(\text{total number of contacts})}{N_p}$</td>
</tr>
<tr>
<td>Time-averaged $CN$ ($&lt;CN&gt;$)</td>
<td>$&lt;CN&gt; = \sum_{i=1}^{N} CN_i/N$</td>
</tr>
<tr>
<td>Average height ($Y_{CM}$)</td>
<td>$Y_{CM} = \sum_{i=1}^{N_p} y_{p,i}/N_p$</td>
</tr>
<tr>
<td>Average axial velocity ($V_{CM,y}$)</td>
<td>$V_{CM,y} = \sum_{i=1}^{N_p} v_{p,i}/N_p$</td>
</tr>
<tr>
<td>Axial bubble granular temperature ($\Theta_{yy}$)</td>
<td>$\Theta_{yy} = &lt;V'_yV'_y&gt;$</td>
</tr>
<tr>
<td>Velocity fluctuation ($V'_y$)</td>
<td>$V'_y = V_y - &lt;V_y&gt;$</td>
</tr>
</tbody>
</table>

Note that in the calculation of $CN$, we assumed that each contact is shared only by two particles. The $CN$ defined here is the same as the ensemble-averaged coordination number calculated in [36] and is representative of the bulk scale compactness of the bed. This measurement is used in this work to quantify the behavior of the solid-phase with the pulsation parameters. At each time step, the instantaneous particle axial velocity, $V_y$, is calculated by averaging the axial velocity of particles, $v_{p,i}$, that are contained in cells with a length in the $x$ and $y$ direction of 4 mm.

The number and size of bubbles were evaluated from $\phi$, using MATLAB’s image processing toolbox [70]. With the average area of bubbles ($A_b$), we calculated the equivalent bubble diameter, $d_b = \sqrt{4A_b/\pi}$. Note that a region is considered as part of a bubble if it contains at least three grid cells with $\phi \leq 0.2$. Finally, two pressure signals are collected:
one from the bottom-center of the bed at a height equal to 1 mm, characterizing the pressure drop over the bed, and the other from the middle-center of the bed at a height of 40 mm.

3.3 Results

3.3.1 Cases Without Pulsation

Figure 3.2 illustrates the type of fluidization occurring at $V_M = 1.1$ and $V_M = 1.3$, through snapshots of the particle volume fraction field, $\phi$.

As observed, a bubbling regime is present in all cases. The increase of $V_M$ produce an enlargement of the bubbles from an equivalent diameter of 5.5 to 8.0 mm. Similarly, the standard deviation also increases, from 1.4 to 2.8 mm, indicating that larger $V_M$ induces the system to experience broader ranges of bubble sizes. These values were obtained for the top half of the bed ($40 \text{ mm} \leq y \leq 80 \text{ mm}$) to highlight the difference in bubble size specifically when bubbles reach the surface of the bed. Figure 3.3 shows the power spectrum distribution (PSD) of the pressure drop signal for each case.
The PSD shows that the pressure signals can be characterized by distinguished frequencies of oscillation, whose values go from 3 to 3.5 Hz as $V_M$ increases. These distinguished peaks are in good qualitative agreement with the characteristic dynamic behavior observed in bubbling micro-fluidized beds [20]. In this numerical work, only internal phenomena to the particle bed are relevant to the fluctuating behavior of the pressure drop signal, i.e. bubble formation, passage and eruption. In particular, eruption of bubbles plays a dominant role among these three [9, 73]. This suggests that the relatively high strength of the peak at 3.5 Hz is a reflection of the higher pressure amplitudes caused by bigger and more developed bubbles in the top region of the bed. For the cases with pulsation, we chose the frequency of the imposed oscillation to be 3.5 Hz.

3.3.2 Cases With Pulsation

Overview of Parametric Space and Flow Field

Figure 3.4 shows a qualitative description of the different behaviors observed for the set of parameters studied in this work. Four distinguishing behaviors or patterns were identified and, correspondingly, a profile of the particle volume fraction in the bed is shown to depict the characteristic features. The dotted line represents the conditions at which the base flow, $V_M - V_A$, is reduced to the minimum fluidization velocity. Below is a description qualifying each pattern based on animation movies of the system:

(△) - high stability - This flow pattern is characterized by regular staggered forma-
Figure 3.4. Parametric space for cases with pulsation investigated in this work. Each symbol indicates the type of flow pattern encountered: (Δ) - high stability; (□) - intermediate stability; (♦) - low stability; and (♦) - formation of void layer through coalescence.

- High stability (Δ): The staggered behavior is observed and occurs throughout the simulation, with no deviation of bubble position. However, occasional changes in pattern type are observed, such as 2-2 type of patterns deviating to 1-2-1 type during the simulation.

- Intermediate stability (□): The staggered formation of bubbles is observed only briefly, without persistence. In some cases, bubbles emerge directly below existing ones, and in others, bubbles align with each other.

- Low stability (♦): This pattern is characterized by the formation of small void structures from the base of the bed, as opposed to a regular formation of a coherent void layer at the base. Bubbles end up coalescing farther up in the bed into a horizontal void layer, which subsequently breaks up into larger bubbles.

The flow patterns may be assessed quantitatively by inspecting the bubble granular
temperature profiles at different heights in the bed (40, 60 and 80mm). Let us look at three cases with decaying stability. Figure 3.5 shows these profiles for the cases with constant $V_A = 0.3$ and varying $V_M = 1.1, 1.2$ and 1.3 (A, B and C).

![Figure 3.5](image_url)

**Figure 3.5.** Plots show the axial bubble granular temperature ($\Theta_{yy}$) at three different heights: 40 (black ●), 60 (blue ■) and 80 mm (red ▲). Plots A, B and C correspond to the pulsation parameters: $V_M = 1.1, 1.2$ and 1.3, respectively, with constant $V_A = 0.3$.

All plots show distinct regions of higher granular temperature. They represent the
preferential paths as bubbles rise in the bed. Plot (A) clearly shows the presence of four peaks, which increase in intensity at higher positions. This has to do with the evolution and development of bubbles and the consequent level of disturbance caused by them. In particular, plot (A) depicts the granular temperature profiles for the case where a 2-2 type of pattern is observed. Two bubbles emerge as the flowrate is oscillated, alternating their position from where the first and third peaks of granular temperature are located to the second and fourth peaks (see profile in Figure 3.4). It is important to note that all the troughs of the granular temperature profile remain at low values even at higher positions. This is related to the easier collapse of the emerging void layers at lower $V_M$ (discussed more in next sections; see Figure 3.20, for example).

In plots (B) and (C), it is possible to observe that this behavior deteriorates: there is an overall increase of the granular temperature even at the troughs. The particle volume fraction profiles shown in Figure 3.4 may be used to exemplify the discussion. The case where $V_M = 1.2$ and $V_A = 0.3$ shows a new emerging void layer with two nucleation sites at its extremes. The reduction in suppression of the void layer allows the middle section to persist, causing the disturbance of regions that are not in the path of bubbles. This is why we see an overall increase in bubble granular temperature. In addition, these reminiscent void structures also add to the deviations observed in staggered patterns as they tend to evolve into bubbles as the superficial velocity increases. Nevertheless, three peaks are observed for cases (B) and (C) specially at 80 mm, that is, a larger wavelength of bubble formation is favored by increasing $V_M$. Even at $V_M = 1.3$, bubbles continue to choose preferential paths; however, the results suggest that, at higher $V_M$, bubble interaction becomes a relevant mechanism for such behavior, inducing alignment of bubbles.

The peaks in granular temperature profile do not necessarily mean a staggered behavior. This can be seen in Figure 3.6 where the behavior previously observed in Figure 3.5A and C are compared. For each condition, the particle volume fraction was probed at two locations, which correspond to the position where the first and second peaks of granular temperature occur in plots (A) and (C) of Figure 3.5. Figure 3.6.A shows the
alternating behavior of the passage of bubbles at the two locations; this is the 2-2 pattern behavior mentioned above. While, Figure 3.6.B indicates a seemingly random behavior.

**Pressure Signals**

Figure 3.7 shows the time-averaged, the averaged minimum and maximum pressure drops in plots A, B and C, respectively. Overall, the trend of the time-averaged pressure drop is an increase followed by a drop. Figure 3.7 indicates that this reduction in pressure drop becomes more pronounced for lower $V_M$ to the extent that, at $V_M = 1.1$, the average pressure drop, at $V_A = 0.4$, is less than the one for pulsation-free conditions. It is important to point out such feature of the average pressure drop as it represents a transition in the behavior of the bed. For the minimum pressure, initially there is a slight decrease
followed by a sharper drop, which is mildly accentuated by the decrease in $V_M$. As to
the maximum pressure drop, the overall trend is of an increase. The case with $V_M = 1.3$
presents a linear relationship with $V_A$, which is disrupted by decreasing $V_M$.

In terms of fluctuations, the pressure drop signal follows very closely the imposed
oscillation of the inflow velocity, such that for all cases with pulsation the main peak in
the PSD is at frequency 3.5 $Hz$. Next is an example for all cases at $V_A = 0.3$ in Figure 3.8.
Other relevant peaks emerge in the PSD of a pressure signal collected from the middle
of the bed, $(x,y) = (80,40)mm$.

Figure 3.9 shows the power spectrum distribution of pressure for all cases with pulsa-
tion, with $V_A$ from 0.1 to 0.4. The main peak in all figures is associated to the imposed
velocity oscillation at a frequency of 3.5 $Hz$. As expected the intensity increases with
velocity amplitude, although we see a slight decrease for the case with $V_M = 1.1$ as we
transition from $V_A = 0.3$ to 0.4. The cases termed highly stable in Figure 3.4 all present
a clear peak at the sub-harmonic frequency, 1.75 Hz. This is a feature of pattern forming
systems with alternating behavior [58]. The presence and intensity of peaks located below
3.5 $Hz$ is mainly related to the eruption of bubbles at the surface; although, at $V_M = 1.1$, passage of bubbles start to play an important role. This will be discussed more in
the next sections.

Particle Volume Fraction

We move on to see the behavior of the void fronts as they rise in the bed against the
velocity amplitude. This is done by averaging the particle volume fraction at three
heights, 20, 40 and 80 $mm$. The passage of the void front is characterized by a drop in
the time series of the particle volume fraction. Figure 3.10 shows the behavior for the
cases under $V_M = 1.1$ and $V_A = 0.1$ (A) and 0.4 (B), as representative cases.

The two plots show that, as $V_A$ is increased, the void front takes less time to reach the
surface of the bed. By cross correlating the signals from 20, 40 and 80 $mm$, it is possible
to estimate the travel time of these void fronts. Figure 3.11 shows the time lag between
each of them.

The overall time for the void front to travel to the surface of the bed (20 to 80 $mm$)

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Figure 3.7. Time-averaged (A), averaged minimum (B), and averaged maximum (C) pressure drop against velocity amplitude ($V_A$) for $V_M = 1.1$ (black ●), 1.2 (blue ■), and 1.3 (red ▲).
Figure 3.8. Time series and power spectrum distribution for pressure drop signals at $V_A = 0.3$ and $V_M = 1.1$ (black), 1.2 (blue) and 1.3 (red).

Figure 3.9. Power spectrum distribution of pressure signal from $(x,y) = (80,40)$ mm. Plots A, B, C, and D correspond respectively to $V_A = 0.1$, 0.2, 0.3 and 0.4; while the line colors, black, blue and red, correspond to $V_C = 1.1$, 1.2 and 1.3.
Figure 3.10. Time series of averaged particle volume fraction at three heights: 20 (black), 40 (blue) and 80 (red) mm. Plots A and B correspond respectively to the following pulsation parameters: $V_A = 0.1$ and 0.4, both at $V_M = 1.1$. 

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Figure 3.11. Time lag between void fronts at 20 and 40 mm (●), 40 and 80 mm (■), and the sum of times (▲). Plots A, B and C correspond respectively to pulsation parameters: $V_M = 1.1$, 1.2 and 1.3. Horizontal line marks one period of the imposed oscillation.

represented by the triangles, tends to decrease with $V_A$ for all cases of $V_M$ (plots A, B and C). While there is a decrease in time for the void fronts to travel from 20 to 40 mm (circles) for all cases, the time for them to travel from 40 to 80 mm (squares) seems to stagnate as $V_M$ is increased. This causes the drop of the overall time to behave sharper for $V_M = 1.1$ than for $V_M = 1.3$, falling below the black line, which represents one period
of imposed oscillation. For all cases of mean superficial velocity, the void layer accelerates as it travels from the middle (40 mm) to the top (80 mm) of the bed. This is because the void fronts travel as bubbles from the middle to the top in contrast to void layers in the first section of the bed. Such acceleration is enhanced with the increase in $V_M$, specifically at $V_A = 0.1$ and 0.2.

The evolution of the void fronts may also be analyzed by the power spectrum distribution of the averaged particle volume fraction time series. We take the cases at $V_M = 1.2$ as representative cases.

Figure 3.12 shows that the void front passes the height of 20 mm at a well-defined frequency of 3.5 Hz for all $V_A$. At this point, the void front is still a single void layer. At 40 and 80 mm, the void front has disintegrated into bubbles and the PSD in Figure 3.12 shows a second peak at frequencies lower than 3.5 Hz. This has to do with the periodical
behavior in the suppression of the void layer. This is easy to see for the case of a 1-2-1 type of pattern. The signal for the passage of the void front composed of two bubbles will be more intense (or have a stronger drop) than the void front with just a single bubble. This periodical behavior is what is being captured by the second peak in Figure 3.12 and is also reflected in the pressure PSD. Take, for example, the case described by \((V_M, V_A) = (1.2, 0.2)\). Figure 3.13 shows the time series of the averaged particle volume fraction at the middle and top of the bed in plots (A) and (B), respectively. The time series clearly show moments of strong and weak drops. The period between two strong drops of particle volume fraction correspond to the frequency described by the secondary peaks in Figure 3.12; while, the period between a strong and weak drop is described by the 3.5 Hz frequency.

The position of the secondary peaks in Figure 3.12 correspond to the position of the
peaks at lower frequencies in the pressure PSD for $V_M = 1.2$ in Figure 3.9. For the cases with $V_M \geq 1.2$, the results indicate that the eruption of bubbles is the dominant mechanism causing the oscillations of pressure described by the secondary peaks in Figure 3.9. For example, for the case described by $(V_M, V_A) = (1.3, 0.2)$, the PSD of the averaged particle volume fraction at 80 mm shows a secondary peak at 2.25 Hz, corresponding to the secondary peak in the pressure PSD; while, the local particle volume fraction oscillations at $(x, y) = (80, 40)$ mm returns a 1.75 Hz dominant behavior. At $V_M = 1.1$, the local passage of bubbles seem to have a larger influence on the pressure oscillations. For example, for the case described by $(V_M, V_A) = (1.1, 0.3)$, the PSD of the averaged particle volume fraction at 80 mm shows a secondary peak at 2.24 Hz, while the dominant frequency of the local particle volume fraction oscillation is 1.75 Hz, which matches the pressure PSD.

**Bed Height**

Let us turn to a description of how the solid phase behaves. Figure 3.14 shows the time-averaged height of the particles and the average of the minimum and maximum heights against $V_A$ in plots A, B and C, respectively.

The average height, plot (A), presents an overall increasing trend. Although, a slight change in slope is observed for cases with $V_M = 1.3$ and 1.2. There is a more prominent change in the case of $V_M = 1.1$. The average remains the same, when it transitions from $V_A = 0.2$ to 0.3. We see a very well behaved growth of the maximum height with $V_A$ in plot (C). However, a more complicated behavior appears for the minimum height in plot (B). There is a transition from a growing slope to a decaying one, which clearly occurs with more strength for the case with $V_M = 1.1$. Such drop is what causes the average, in plot (A), to remain the same. Let us look more closely to the time series of the case with $V_M = 1.1$ in Figure 3.15.

The particle bed is mainly pushed up as $V_A$ goes from 0 to 0.2. Note that, for cases with $V_A = 0.1$ and 0.2, their minimum values barely go below the values of the case with $V_A = 0$. Once $V_A = 0.3$ is achieved the system starts to access lower heights when compared to the other conditions, settling almost completely.
Figure 3.14. Time-averaged (A), averaged minimum (B), and averaged maximum (C) height of the particle bed against velocity amplitude ($V_A$) for $V_M = 1.1$ (black ▪), 1.2 (blue ■), and 1.3 (red ▲).

The initial behavior resembles the case at higher imposed frequencies of oscillation where the bed is not allowed to completely settle. However, the frequency is maintained constant and new void layers are formed at each cycle. This result suggests that the solid phase is being able to suppress more strongly the emerging void layers with the increase in $V_A$. This enables it to compact almost entirely; thus, the lower heights.
Figure 3.15. Time series of the particle bed height at $V_M = 1.1$ for $V_A = 0$ (blue), 0.1 (orange), 0.2 (yellow), 0.3 (purple) and 0.4 (green)

Coordination Number

Figure 3.16 shows the change in time averaged coordination number, $<CN>$, with $V_A$.

As expected the bed exists under a more compact state at smaller $V_M$. The trends follow a similar behavior as the one for the pressure drop with the increase in $V_A$. As can be seen, the addition of oscillations to the inflow firstly increases the overall bed compactness, reaching a maximum value, which is then followed by a drop. Such drop is accentuated with the decrease in $V_M$. For example, compare $<CN>$ at $V_A = 0$ and 0.4 for each case of $V_M$. 

Figure 3.16. Time-averaged coordination number ($<CN>$) for all $V_A$ values at $V_M = 1.1$ (●), 1.2 (■) and 1.3 (▲).
Next, in Figure 3.17, we look at the time series and histograms of the coordination number for the case with $V_M = 1.1$ and $V_A = 0.1, 0.2, 0.3$ and 0.4.

Figure 3.17. Time series (1) and histogram (2) of normalized coordination number (0 mean and 1 standard deviation) at $V_M = 1.1$ with $V_A = 0.1$ (A), 0.2 (B), 0.3 (C) and 0.4 (D).

The plots of $CN$ indicate that the transition observed for $<CN>$ in Figure 3.16 is
marked by a change in the dynamics of the solid phase. In fact, as observed in the histograms, the system switches to a dynamics in which the particle bed spends more time under low $CN$. The plots also indicate that this behavior has to do with a second drop in coordination number at the trough of the time series. Such behavior may be thought to occur because of an extended expansion of the bed. However, as Figure 3.18 indicates, the solid phase passes through this second valley as it is coming down from its expanded state.

![Figure 3.18](image)

Figure 3.18. Time series of coordination number and average axial velocity of the particle bed at $V_M = 1.1$ and $V_A = 0.4$. The horizontal black line indicates when axial velocity is zero and the vertical indicates when a second drop in coordination number is about to start.

It is possible to see in Figure 3.18 that the average axial velocity for the system is negative when the second valley in $CN$ time series occurs. If particles are moving downwards, the total volume occupied by the particle bed is decreasing. Therefore, the second drop in $CN$ means that particles are moving to the lean-phase at this moment, which consequently implies that the emerging void layers are being suppressed. The collapse of the emerging void layer particle roof allows the dense-phase on top of it to experience a decompression as the space occupied by gas in the void layer is replaced with particles. Figure 3.19 shows comparisons of the void front that passes in the middle of the bed for $V_A = 0.1$, 0.2, 0.3 and 0.4 at $V_M = 1.1$.

Plot (A) shows the intensity of the void fronts for cases with $V_A = 0.1$ (black) and 0.2 (blue). The solid lines connect the minimum values in the plot. It is possible to see
Figure 3.19. Time series of average particle volume fraction at height 40 mm for cases with $V_M = 1.1$. Solid lines connect the minimum values. Plots A, B and C present comparisons between cases with $V_A = 0.1$ (black) and 0.2 (blue); 0.2 (black) and 0.3 (blue); and 0.3 (black) and 0.4 (blue), respectively.
that there is a decrease in the particle volume fraction of the fronts with an increase in $V_A$. The average value of the minimum points goes from 0.47 to 0.43. In plot (B), however, we see the opposite behavior: with the increase in $V_A$, from 0.2 (black) to 0.3 (blue), there is an increase in the particle volume fraction; the averaged minimum goes from 0.43 to 0.49. Lastly, in plot (C), the behavior persists, but only a slight increase is observed, from 0.49 to 0.51. These changes follow the transition observed in $< CN >$ and suggest an increased suppression of the void layer at $V_A = 0.3$ and 0.4.

The results indicate that the behavior observed for $CN$ diminishes with the increase in $V_M$ (or the base flow $V_M - V_A$), holding $V_A$ constant, as observed in Figure 3.20. This suggests that the collapse of the void layer is more effective at lower $V_M$. On the other hand, Figure 3.21 indicates that the effect of changing $V_A$ at a constant base flow, $V_M - V_A$, is less disruptive of the dynamics of the solid phase.

### 3.4 Discussion

All the measurements indicate that the system undergoes a transition when $V_A$ is increased while holding $V_M$ constant, with most abrupt changes occurring at the lowest $V_M$. In summary, such transition is marked by: (1) a peak in time-averaged pressure drop and coordination number; (2) a change in the dynamics of the solid phase; (3) an increase in the velocity of the void fronts traversing the particle bed and (4) a decrease in the minimum average height attained by the solid phase. The following is a brief discussion on how these changes relate to each other.

As was explained, the second valley in the trough of the coordination number time series (Figure 3.17) occurs as the particle bed is moving downwards (Figure 3.18), which precludes the alternative explanation, wherein the system is being further expanded. This implies that the void layers are collapsing due to the stronger intensity with which the whole bed settles. Therefore, the change in the dynamics of the coordination number (Figure 3.17) is an indication of a better suppression of the void layers. That also explains why the solid phase reaches lower heights (Figures 3.14.B and 3.15). In addition, this also influences the rise velocity of the void structures (Figure 11), since, with a stronger collapse, the void fronts form sparse bubbles, instead of remaining and rising as slugs.
Figure 3.20. Histogram of normalized coordination number (0 mean and 1 standard deviation) at $V_A = 0.3$ with $V_M - V_A = 0.8$ (A), 0.9 (B) and 1 (C).
Figure 3.21. Histogram of normalized coordination number (0 mean and 1 standard deviation) at $V_M - V_A = 0.8$ with $V_A = 0.3$ (A), 0.4 (B) and 0.5 (C).
We attribute two reasons to the initial increase in pressure drop. The first reason is an increased segregation of dense and lean phases, which may be concluded from Figures 3.14, 3.15 and 3.16: even though the bed has a larger averaged height, its time-averaged coordination number increases. The second reason is that the void structures start to rise in the bed as void fronts, causing the system to behave similarly to slugging fluidized beds. In this case, the sharp pressure gradient in the wake of erupting bubbles is the dominant mechanism for pressure fluctuations and influences the pressure drop [12]. Thus, the combined effect of larger bubbles travelling as void fronts with denser wake regions induces an increase in time-averaged pressure drop. On the other hand, the stronger collapse of incoming void layers at higher $V_A$ generates sparse bubbles. This causes a reduction of the high pressure gradient wake region at the eruption moment, which induces a reduction in the average pressure drop. At higher $V_M$, however, the void layer is able to resist the settling of the solid phase. In this case, the generated bubbles fill almost completely the horizontal extension of the bed (see the profile of case $(V_M, V_A) = (1.3, 0.5)$ in Figure 3.14), causing the reduction in pressure drop to behave in a more gradual fashion with $V_A$.

It is worth highlighting the capability of the average coordination number in assessing the dynamics of the solid phase (Figure 3.17). In many situations, a lower time-averaged coordination number (Figure 3.16) is desirable. However, Figures 3.20 and 3.21 show that this can be achieved through different routes: either by increasing the base flow, $V_M - V_A$, and keeping $V_A$ constant, or by increasing $V_A$ with constant $V_M - V_A$. Both changes lead to an overall reduction of time-averaged coordination number, but the dynamics of the bed is affected in such a way that longer periods at lower coordination number is maintained by the latter change, while, disrupted, by the former change. This is specially important to establishing the best conditions for partial pulsation systems where the base flow, $V_M - V_A$, can be adjusted.

3.5 Conclusion

In this work, we performed a numerical investigation of the behavior of a pseudo-2D pulsed-fluidized bed consisting of Geldart B particles. Computational Fluid Dynamics
and Discrete Element Method were utilized in conjunction to obtain detailed information about the dynamics of the particle bed, focusing on its response to variations of the mean gas velocity, $V_M$, and the amplitude of oscillations, $V_A$. Initially, a pulsation-free system was investigated to understand its natural behavior. Then the effects of pulsation were analyzed holding the imposed frequency at $3.5 \text{ Hz}$.

Next, we list conclusions of this work:

- The bed manifested different flow fields depending on $V_M$ and $V_A$:
  - The increase in $V_A$ induced the system to go from a bubbling regime to a situation where void layers are formed at the bottom of the bed and disintegrate into bubbles as they rise.
  - At $V_M = 1.1$, highly stable staggered formation of bubbles was observed and pressure measurements from the middle of the bed correctly identified them with a peak at subharmonic frequency, $1.75 \text{ Hz}$.
  - The disintegration process of the void front into bubbles varies periodically and is captured by the power spectrum distribution of the particle volume fraction.
  - The preferential paths of the bubbles was demonstrated with the bubble granular temperature profile.
  - The results indicate that higher $V_M$ may induce patterns with larger wavelengths.

- The pulsed fluidized bed undergoes a regime transition as $V_A$ is increased, holding $V_M$ constant:
  - The results indicate that this transition is caused by stronger suppression of the emerging void layers with the increase in $V_A$.
  - The transition is underlined by: (1) a peak in time-averaged pressure drop and coordination number; (2) a change in the dynamics of the solid phase; (3) an
increase in the velocity of the void fronts traversing the particle bed and (4) a decrease in the minimum average height attained by the solid phase.

- The transition occurs in a more gradual fashion at higher $V_M$ due to the increased strength of the void layers to resist the collapse of the solid phase.

- The average coordination number of the system is able to capture the shift in dynamics of the solid phase, enabling its use to identify what changes to pulsation parameters are most disruptive to the system:
  - The increase of base flow, $V_M - V_A$, with constant $V_A$ is more disruptive of the stronger suppression of the void layer than the increase of $V_A$ at constant $V_M - V_A$.

This work helps guide the use of pulsation parameters in achieving an optimized behavior of pulsed fluidized beds as well as in the reading of future experimental results in systems where visualization is not possible. Although, much more information is needed to characterize such transition and its response to changes in particle and fluid properties as well as bed geometry.
Chapter 4. Wall-induced Hydrodynamic Forces

4.1 Introduction

Hydrodynamic forces arise from the interaction between fluid and solid phases. Their quantification is a key component in the correct prediction of the dynamics and evolution of particle-laden flows, with many factors contributing to their variability. The presence of a stationary wall is one such factor of relevance for both environmental and industrial flows. For example, the interaction of suspended sand and the seabed plays a crucial role in sediment transport mechanisms occurring in coastal zones [84, 83]. Transport of particles in industry occur mainly in bounded equipment, which affects the flow pattern of particles, e.g., slurry reactors [24, 99] and pneumatic conveyors [48]. Additionally, wall effects have gained considerable importance in the development of new microfluidic devices [67]. Thus, further understanding of wall-induced hydrodynamic interactions is paramount for comprehending natural phenomena as well as for the design of industrial equipment.

As a canonical flow system, the fixed single sphere hydrodynamics serves as a starting point for considering the effects of the wall. It is well known that the flow field in the wake of the sphere undergoes three main transitions until transient behavior [45, 88]. Firstly, at $Re \approx 20$, the flow field separates from the sphere, forming an axisymmetric vortex ring in its wake. Such behavior continues until $Re \approx 211$, where the symmetry breaks down, leading to the opening of the vortex structure. In this case, planar symmetry still exists and develops spontaneously as a result of intrinsic instabilities in the flow field. Additionally, this developed asymmetry induces the sphere to experience a lift force. At $Re \geq 270$, a time-dependent wake arises, eventually leading to a periodical shedding of vortices in a peculiar fashion, resembling hairpins.

Such structures and transitions are altered by the presence of other particles. The understanding gathered from multiple particle hydrodynamic interactions of fixed equal spheres in uniform unbounded flow is valuable in the interpretation of the scenarios where walls are present. In-tandem and side-by-side arrangements of two spheres are the most commonly explored configurations. Previous works have reported on variations of
hydrodynamic forces and flow structures as a function of Reynolds number and separation distance between the spheres. The following are key features of previous studies:

- In the tandem arrangement, the trailing sphere experiences significant reduction in drag force, which may be described by a power law of the separation distance [117, 81].

- At $Re \leq 150$, repelling or attractive lift forces emerge as a function of separation distance in the side-by-side configuration [47, 26]. This behavior seems to cease at $Re = 300$ [109].

- In both configurations, separation distance may induce or delay flow structure transition typical of a non-interacting sphere. Additionally, new flow features may emerge as a result of wake interaction. For example, double-sided vortex shedding is reported in a side-by-side configuration at $Re = 200$ when particles are almost touching [91, 90, 118].

In addition to these two arrangements, flow and force maps have been developed for all possible configurations for $Re \leq 300$, adding another degree of freedom, the angle between the line connecting the spheres and the incoming flow [81, 109, 108, 3]. Furthermore, systems with more than two spheres in various configurations have been investigated [62, 16, 65, 49, 17, 82].

Under moderate Reynolds numbers, the following series of papers have systematically investigated the wall effect by gradually considering sphere-wall situations of higher complexity. Different elements of the motion of a sphere, such as translation and rotation, were combined with different effects of a nearby wall, such as its mere presence and induced shear flow. Different forces arise due to the presence of the wall, which may be classified as translation-induced (wall+sphere translation); rotation-induced (wall+sphere rotation); and shear-induced (wall+shear flow). Zeng and Balachandar (2005) investigated the wall-induced hydrodynamic forces on a sphere under no-shear conditions. The sphere was towed along the wall at four separation distances, from 0.75 to 4 sphere diameters, for $0.5 \leq Re \leq 300$. Their work showed that the distance from the wall modulates the
critical Re at which transitions of flow field structures occur and, consequently, the hydrodynamic forces experienced by the nearby translating sphere. For example, such study revealed a down-and-up trend of the lift coefficient at Re $\approx$ 100, which was correlated to the appearance of a double-threaded vortex structure. Additionally, the onset of unsteadiness was accelerated at large to intermediate distances, but was significantly delayed at close proximity. Later, the effect of linear shear flow in a wall-bounded configuration was considered within a wider range of distances from the wall with a case of a nearly-touching sphere (0.505 sphere diameter). Under this latter condition, both drag and lift forces magnitude is enlarged in comparison to the simply translating sphere scenario in the previous study. The effects observed for the hydrodynamic forces were compared with theoretical predictions and summarized into correlations of Re and distance from the wall [113]. Previous results were extended to the case of a sphere in arbitrary translational and rotational motion in a wall-bounded linear shear flow in [53]. Initially, the authors looked at the effect of sphere rotation in a wall-bounded configuration for a rotational Reynolds number, $1 \leq Re_\omega \leq 100$, at different separations from the wall, from 0.505 to 4 sphere diameters. In this case, the wall breaks the axisymmetry, along the rotation axis, of the spiralling flow and induces a non-zero drag force on the sphere due to shear stress differences between the gap region below the sphere and region above it. Their results showed that rotation-induced drag and lift forces are comparably weak to the shear and translation-induced ones. They further investigated the binary contributions coming from shear-translation, shear-rotation and translation-rotation interactions to the lift and drag forces. Then, by assuming the validity of superposition of such coupling terms obtained in low-Reynolds-number conditions [50], they proposed functional forms for the composite drag and lift forces and computed correction factors to them based on numerical simulations that considered two mechanisms at a time. These composite correlations were tested against direct numerical simulations in a later work [55]. Based on previous studies in unbounded flows, particle-particle hydrodynamic interactions are relevant even under very dilute conditions. For example, dual-particle systems in tandem arrangement with inter-particle separation of 6 diameters may induce as much as 30%
reduction in drag coefficient of the trailing particle. For this reason, significant deviations to the correlations mentioned above are expected, and further investigation of the effects of walls on the hydrodynamic interactions among nearby particles is required.

The study of the effect of stationary walls in a multiple-particle system is spread over different areas of application. For example, the demand for higher throughputs has steered the microfluidics field to take advantage of inertia-activated forces, such as the shear and wall-induced lift forces, for generating lateral passive focusing of particles. Additionally, such hydrodynamic interactions coupled with resulting fluid flow patterns (i.e. reversing flows) were shown to be part of a self-assembly mechanism that leads to the formation of stably aligned particle trains [69, 56, 37]. These phenomena are relevant for systems in biomedicine and material synthesis where high precision and controllability are required. The onset of motion of particles sitting on top of rough walls (substrate) is an important aspect of particle transport in general and has served as a motivation for the understanding of hydrodynamic interactions induced by stationary walls. For example, Derksen and Larsen (2011) randomly generated layers of fixed particles and investigated the r.m.s and average behavior of drag and lift forces for each layer as a function of its concentration and height in the stack. Their results show an overall reduction of drag and lift due to the blockage of fluid flow within the bed. Shielding effects due to partial coverage of free-to-move particles by the substrate particles has also been investigated by considering different substrate spacing, arrangement, and size ratio between the particles composing the substrate and the free-to-move particle [1, 89]. In these cases, particles are in contact with the substrate at low $Re$, and they find that significant deflection of the flow field arise specifically when the sitting particle size is of the same order as of the substrate particles. Overall, the lift force is neglected in their models due to its relatively low magnitude. Conversely, studies under turbulent conditions have indicated the significant role lift forces play in favouring particle dislodgement [14, 60]. Lee and Balachandar (2017) and Li et al. (2019) have continued the numerical investigation described in the previous paragraph. They looked at the effect of roughness of the wall on a single particle under linear shear flow and turbulent conditions, considering a single
particle at different distances from the wall. Overall, they report that the smooth-wall correlations are sufficiently reliable under rough-wall conditions by redefineing some of the characteristic parameters such as the gap distance between the sphere and rough bed and the governing Reynolds number. In the latter study, however, severe deviations are also found: it is shown that the wall-normal force for a fixed suspended particle is mainly caused by wall-normal drag force, implying the inadequacy of the lift correlation developed in [113] for this case.

The goal of the present work is two fold: (1) to demonstrate the capabilities of a recently developed implementation of the distributed Lagrange multiplier method within the Basilisk solver framework [78] and (2) to further the understanding of the wall effect on the hydrodynamic interactions of particles. Although considerable effort has been poured into the subject, detailed information about the effect of the walls in the hydrodynamic interaction of two or more suspended spheres has been scarcely studied. Therefore, we choose to start such investigation with a simple scenario of two fixed spheres in tandem arrangement in translation along a wall. This can be seen as an extension of Zeng and Balachandar (2005) work.

4.2 Methodology

4.2.1 Problem Description

In this work, the flow past two spheres of same diameter, $D$, at a distance $L/D = 1$ from a stationary wall is investigated. The spheres are held fixed at a constant velocity, $-U$, in tandem arrangement, and the effect of interparticle distance, $d/D$, on hydrodynamic forces and flow structures are assessed for Reynolds numbers, $Re = UD\rho_f/\mu_f$, up to 200. This configuration isolates the effect of the presence of the wall on the hydrodynamics of the two-spheres system, and relative motion between the two spheres is neglected. Figure 4.1 shows an schematic of the system in a laboratory reference frame.

4.2.2 Numerical Approach and Validation

A distributed Lagrange-multiplier based fictitious domain method (DLM/FD) is used for the simulation of the flow field around the two-spheres configuration scenario. This approach consists in solving a combined equation of motion, encompassing both fluid and
Figure 4.1. Schematic of two spheres being towed at a constant velocity near a wall particle media, together with the continuity equation; while the rigid-body motion of the solid phase is enforced through constraints relaxed by distributed lagrange multipliers, $\lambda$ [30, 96]. The governing equations in dimensionless and non-variational form is seen next (Equations 4.1-4.5), where the region of the domain occupied by the solid-phase is described by $S$, while the whole domain (fluid plus solid), by $\Omega$:

$$\frac{\partial u}{\partial t} + u \cdot \nabla u + \nabla p - \frac{1}{Re} \nabla^2 u + \lambda = 0 \text{ over } \Omega,$$

$$\left(\frac{\rho_p}{\rho_f} - 1\right)V \frac{dv}{dt} - \int_P \lambda dx = \left(\frac{\rho_p}{\rho_f} - 1\right)V g \text{ over } S,$$

$$\left(\frac{\rho_p}{\rho_f} - 1\right)(I \frac{d\omega}{dt} + \omega \times I \omega) - \int_P r \times \lambda dx = 0 \text{ over } S,$$

$$u - (v + \omega \times r) = 0 \text{ over } S,$$

$$\nabla \cdot u = 0 \text{ over } \Omega$$

The variables $u$, $v$, $\omega$ and $r$ refer to the fluid velocity; the particle translational and angular velocities; and the center-to-surface distance of the particle. For a case with no solid-phase motion, the solution algorithm reduces to two steps: (1) solution of Navier-Stokes and continuity equations (Eqns. 4.1 and 4.5) and (2) solution of the DLM/FD problem (Eqns. 4.2-4.5). In order to decrease computational cost while adequately capturing relevant physics, it is desirable to solve these equations under an adaptive mesh refinement procedure. For this reason, the solution algorithm has been implemented within the Basilisk solver framework: an open source partial differential equation solver on adaptive Cartesian meshes [78]. The Basilisk Navier-Stokes solver is used for the first step. It consists of a second-order implementation in time and space, where advection and
diffusion terms are respectively estimated using Bell-Collela-Glaz and Crank-Nicholson schemes \[8\] within a staggered-in-time projection method. A tree-based approach is used to spatially discretize the domain into finite volumes, and a multigrid solver is used in combination with its hierarchical structure to solve the time-splitted equations. The refinement procedure uses down-sampling (interpolation) and up-sampling (average) of the numerical solution to estimate the error associated with the local discretization. The error estimate is used together with assigned values of maximum level of refinement and error threshold criteria to determine whether refinement or coarsening should take place \[35, 79, 77\].

The DLM/FD step is formally a saddle-point problem, which is solved by the Uzawa-Conjugate gradient iterative method as described in \[95\]. Two important aspects to the accuracy of this step are the distribution of Lagrange multipliers over the solid phase region and the interpolation procedure associated with the reconstruction of flow field at the solid-fluid interface. The Lagrange multipliers are spatially discretized by a collocation method, using Dirac functions as basis functions. For interior cells the multipliers reside in the cell center together with the velocity components, while surface points are distributed based on the generalized spiral set described in \[85\], and a $Q_2$ interpolation operator is used to reconstruct the flow field at these locations. Comparisons with different distribution and interpolation procedures have been performed previously \[96\], showing that the choices made here lead to enhanced results in terms of insensitivity of flow field direction relative to the axis of point distribution and lower error magnitude with respect to the multi-linear interpolation operator. As a result, the Lagrange multipliers are computed and the rigid-body motion accurately enforced within the solid region ($S$). Equations 4.6 and 4.7 may be applied to obtain the hydrodynamic force and torque acting on the solid phase.

\[
F = \int_P \lambda dx + V \frac{dv}{dt}, \quad (4.6)
\]

\[
T = \int_P r \times \lambda dx + J \frac{d\omega}{dt} + \omega \times J \omega \quad (4.7)
\]
Note that for fixed spheres or spheres experiencing a constant motion in time, only the first term in equations 4.6 and 4.7. Drag and lift forces are reported as coefficients, which are calculated as follows.

\[ C_D = \frac{F \cdot e_x}{\left( \frac{1}{8} \rho U^2 \pi D^2 \right)} \]  \hspace{1cm} (4.8)

\[ C_L = \frac{F \cdot e_y}{\left( \frac{1}{8} \rho U^2 \pi D^2 \right)} \]  \hspace{1cm} (4.9)

The domain simulation consisted of a cubic region of size \( 48D \). The leading sphere was fixed at \( x/D = 8 \); while the trailing sphere position was varied such that \( 1.5 \leq d/D \leq 6 \). Previous investigations have shown that the domain size and positions of the spheres are well within conditions to eliminate spurious boundary effects [112, 113]. The front, back and top boundaries were assigned Neumann conditions, \( \mathbf{n} \cdot \nabla \mathbf{u} = 0 \), and an outflow condition (\( p = 0 \)) is assigned to the right (\( x/D = 48D \)) boundary. Similarly to the study of a single sphere by Zeng and Balanchandar (2005), simulations are carried out in a reference frame following the two-sphere system. From this perspective, both the bottom wall (\( y/D = 0 \)) and left boundary (\( x/D = 0 \)) are moving with fixed velocity, \( Ue_x \). The simulations were started under uniform flow everywhere and carried out until steady-state was reached. The maximum \( \Delta t \) used was 0.01, which was automatically adjusted by the Basilisk solver to be small enough such that the CFL number was less than 0.8 throughout the simulation. The error threshold criterion for the flow field velocity was chosen to be \( 2.5 \cdot 10^{-3} \). Additionally, a shell consisting of three grid cells at maximum resolution is enforced in the fluid-solid interface in order to promote a simple implementation of the quadratic interpolation mentioned above. A maximum resolution of \( D/\Delta x = 43 \) and 86 was assigned to the cases where \( Re \leq 50 \) and \( Re \geq 100 \), respectively. Figure 4.2 shows an example of the mesh surrounding the sphere at \( Re = 100 \) for a single-sphere case and the convergence behavior of the drag coefficient.

Validation of the numerical methodology and parameters used was performed against results from spectral element simulations of a single sphere near a wall [112]. Spectral
Figure 4.2. Adaptive mesh surrounding sphere. Convergence trend based on drag coefficient of single sphere at $Re = 100$ against number of cells across particle diameter ($D/\Delta x$).

Table 4.1. Relative error of drag and lift coefficients obtained using Basilisk-DLM/FD implementation with respect to Spectral Element Method results.

<table>
<thead>
<tr>
<th>$Re$</th>
<th>$C_{D,Basilisk}$</th>
<th>$C_{D,SEM}$</th>
<th>$RE$(%)</th>
<th>$C_{L,Basilisk}$</th>
<th>$C_{L,SEM}$</th>
<th>$RE$(%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>4.742</td>
<td>4.717</td>
<td>0.5</td>
<td>0.355</td>
<td>0.351</td>
<td>1.1</td>
</tr>
<tr>
<td>200</td>
<td>0.8109</td>
<td>0.8172</td>
<td>0.7</td>
<td>0.0626</td>
<td>0.0607</td>
<td>3.1</td>
</tr>
</tbody>
</table>

element simulations are high fidelity approaches and serve as a good benchmark for the trustworthiness of our numerical methodology. Additionally, the results obtained for single sphere near a wall are used as reference values for the cases with two spheres. Figure 4.3 shows that both qualitative and quantitative features of the lift coefficient for different $Re$ at $L/D = 1$ are well captured by our approach. Such agreement is not only based on point-wise measurements, but is also demonstrated in the pressure distribution profile over the sphere for $Re = 200$ (Figure 4.4).

A more detailed comparison is presented in Table 4.1, which shows a maximum relative error of 3.1% for the lift force at $Re = 200$. These results demonstrate that the numerical scheme and parameters used are adequate and reliable.

4.3 Results and Discussion

4.3.1 Flow Field

For the cases studied in this work, the flow field can be distinguished into two groups, (1) $Re \leq 10$ and (2) $Re \geq 50$, based on the wake characteristics of the spheres. The wake
Figure 4.3. Comparison of the lift coefficient obtained from Basilisk-DLM/FD and Spectral Element Method ([112]) for different Re at $L/D = 1$.

Figure 4.4. Pressure distribution coefficient over bottom and top of a single sphere at $Re = 200$ and $L/D = 1$.
becomes asymmetric somewhere under the following conditions: $10 < Re < 50$.

For a single sphere near the wall at $Re \leq 10$, the flow continues attached to the sphere without circulation zones. Although, in this case, the stagnation points are slightly shifted toward the wall in comparison with the case of a sphere in unbounded flow. Figure 4.5 shows the streamlines for the case of two spheres at $Re = 10$. At relatively large separation distances, $d/D = 4$, part of the fluid coming from the top of the leading sphere travels to the bottom region of the trailing one (plot D). As separation is decreased there is a shift in this behavior. At $d/D = 3$ (plot C), the fluid particles remain in their respective region as they rejoin in the wake of the leading sphere, and, at $(d/D = 2)$, the fluid passing below the leading sphere is pushed towards the top of the trailing one through the gap between them (plot B). At $d/D = 1.5$ (plot A), it is possible to see the initiation of circulation zones in the gap region, with fluid separating from the bottom of the leading sphere and ascending in a more tortuous path. Taneda (1979) demonstrated that in unbounded flows such separations may occur even in the Stokes regime. At $d/D = 1.7$, experiments showed separation of flow occurring between two spheres in-tandem arrangement at $Re \approx 10^{-2}$.

At $Re \geq 50$, the presence of the wall induces the onset of asymmetry in the wake of a single sphere considered in isolation [112]. Figure 4.6 shows the streamlines for the case of two spheres at $Re = 50$. Initially, at $d/D = 3$ and 4, the circulation pattern in the wake of the leading sphere follows that observed for a single sphere near the wall. Additionally, the topology of the wake as seen in plot (C) is similar to that of spheres put side-by-side at $Re = 100$ [47] and of a single sphere in unbounded flow at $Re = 250$ [45]. The same flow features are observed in the wake of the trailing sphere, however, attenuated by the presence of the leading one. The three-dimensional nature of the flow behind the leading sphere is shown in Figure 4.7. Kim et al. (1993) discussed the flow pattern in the side-by-side case considering only the two-dimensional stream traces as in Figure 4.6. They describe how the separated flow on the side farthest from the second sphere is entrained by the high velocity flow field coming from the gap between the spheres. Later, Johnson and Patel (1999) looked more closely into the mechanism of the non-axissymmetric structure at $Re = 250$. Their results show a different flow pattern.
Figure 4.5. Streamlines around two spheres at $z = 24$ at $Re = 10$ for separation distances $d/D$ equal to (A) 1.5, (B) 2.0, (C) 3.0 and (D) 4.0.
Figure 4.6. Streamlines around two spheres on $z = 24$ at $Re = 50$ for separation distances $d/D$ equal to (A) 1.5, (B) 2.0, (C) 3.0 and (D) 4.0.
behavior in the wake of a non-interacting sphere than what is observed in the wake of the leading sphere in Figure 4.7. As can be seen, the flow that separates from the top of the sphere forms a vortex and is transported azimuthally to a second vortex on the opposite side, at which point it is carried downstream. In their case, two vortices are also present, but the separating flow is first entrained into a vortex on the opposite side for then to be transported azimuthally to the other vortex focus. This difference in flow pattern suggests that, although asymmetric, a different mechanism from what was described in [45] is active, which could be accounted for either by the lower $Re$ studied here or the effect of the wall.

Plot (B) (Figure 4.6) depicts a behavior common to all cases from $Re = 50$ to 200: the three-dimensional nature of the flow pattern between spheres undergoes a significant change in signature and becomes more complicated. Chen and Lu (1999) reported a similar behavior for experiments with two spheres in unbounded flow. Although at $Re < 200$, they describe the flow pattern occurring in between the spheres at $d/D = 2$ as random and turbulent. In this case ($Re = 50$ and $d/D = 2$), two circulation zones are observed as in larger separations. However, the flow field coming from the bottom separates from the leading sphere and creates a circulation zone attached to the sphere. Part of the flow coming from the bottom of the leading sphere splits into two streams: one moves directly to the top of the trailing sphere, while the other returns and circumscribes the top vortex. Note also the elongation of the wake of the leading sphere at $d/D = 2$. 

Figure 4.7. Three dimensional fluid particle path in the wake of the leading sphere at $Re = 50$ and $d/D = 3$. 
Such behavior has also been reported in previous works [62, 90] in unbounded flow. At $d/D = 1.5$ (plot (A)), the flow follows an s-shaped path towards the top of the trailing sphere, and fluid particles travel azimuthally from the bottom circulation zone to the top one. Such behavior is similar to what was observed for the case of $Re = 10$, although with more developed circulation zones. The case with $Re = 100$ shows the same flow topology as depicted in plots (A), (C) and (D).

As expected the increase to $Re = 200$ causes an extension of wake region of the spheres. In Figure 4.8, plots (D) and (C), it is possible to observe that the wake of the leading sphere shows the same flow pattern as that of a non-interacting sphere in the unbounded flow at $Re > 211$. Note that the asymmetric and extended wake region causes the front stagnation point of the trailing sphere to shift significantly to the top. This has an effect on the hydrodynamic forces experienced by the trailing sphere as discussed in subsequent sections and is relevant even in large distances, $d/D = 6$. As mentioned before, the flow pattern seems to undergo a significant transition at $d/D = 2$, gaining a more symmetric profile at $d/D = 1.5$ as in the cases with lower $Re$. At $Re = 150$, the topology of the flow is as shown in plots (A), (C) and (D).

Figure 4.9 shows the $z$-component of vorticity for the cases of $Re = 10$, 50 and 200 in rows 1, 2 and 3, respectively. Overall, the effect of $Re$ is immediately seen: (1) top-bottom asymmetry is accentuated along the streamwise direction; (2) stronger vorticity is carried farther away downstream; and (3) thinning of vorticity layer. The higher velocity condition in the gap between leading sphere and wall causes the asymmetry to emerge. The reduction in $d/D$ as was shown previously induces changes in the flow field in the gap between spheres. Note, at $Re = 200$ and $d/D = 3$, the shift in sign of vorticity occurring at the top of the trailing sphere, corresponding to the asymmetric wake in plot (C) of Figure 4.8. With the decrease in $d/D$, vorticity distribution in the gap region reduces in intensity and becomes more symmetric.

4.3.2 Vortical Structures

In this section, the vortical structures at certain conditions are investigated. This is done by utilizing the definition given by Jeong and Hussain (1995), wherein a vortical structure
Figure 4.8. Streamlines around two spheres on $z = 24$ at $Re = 200$ for separation distances $d/D$ equal to (A) 1.5, (B) 2.0, (C) 3.0 and (D) 4.0.
Figure 4.9. Z-component of vorticity on $z = 24$ at $Re = 10$ (1), 50 (2) and 200 (3) for separation distances $d/D$ equal to (A) 1.5 and (B) 3.0.

is defined as a connected region containing two negative eigenvalues of $S^2 + \Omega^2$. $S$ and $\Omega$ are the symmetric and antisymmetric parts of the velocity gradient tensor. A sufficient condition for this is that the second largest eigenvalue, $\lambda_2$, be negative. The streamlines in Figures 4.6 and 4.8 depicted a shift in behavior occurring at $d/D = 2$, with an increase in the complexity of the flow pattern at this separation distance. The effect of $Re$
at this condition on the vortical structures are seen in Figure 4.10 through isocurves of $\lambda_2$.

Figure 4.10. Isocurves of $\lambda_2 = -0.01$ on $z = 24$ at $Re = 50$ (A), 100 (B), 150 (C) and 200 (D) at $d/D = 2$.

Overall, the trailing sphere possesses a significantly different $\lambda_2$ profile as compared to the single sphere case. The toroidal structure engulfing its middle section resembles the profiles at lower $Re$ [113], indicating the attenuation caused by the leading sphere. On the other hand, the upper half $\lambda_2$ profile of the leading sphere closely resembles those of a single sphere in unbounded flow [45]. Specifically, the effect of $Re$ is observed in two ways. For the trailing sphere, the extension of the vortical structures is increased in the wake of the trailing sphere, which leads to a double-thread structure at $Re \approx 100$. For the leading sphere, an enlargement of the top vortical structure and a suppression
of the bottom one is observed with an increase in $Re$. This behavior is correlated to the variation in lift force experienced by the trailing sphere. The three-dimensional nature of the structures are depicted for the case of $Re = 200$ in Figure 4.11.

![Figure 4.11](image)

Figure 4.11. Isosurfaces of $\lambda_2 = -0.01$ at $Re = 200$ for $d/D = 1.5$ (A), 2.0 (B), 3.0 (C).

The trailing sphere presents a double-thread structure for all distances shown in Figure 4.11. Plot (C) shows that the double-thread segments in the wake of the leading sphere are compressed by the presence of the trailing one. At $d/D = 2$, this structure is completely eliminated. The side view with corresponding isocurves on $z = 24$ offers another perspective into the transition occurring within these distances, $1.5 \leq d/D \leq 3.0$.

Figure 4.12 shows that, from $d/D = 3$ to 2, the trailing sphere suppresses the vortical structures located in the middle-bottom of the leading sphere wake. With further decrease in $d/D$, vortical structures in this region reemerge, creating a more symmetrical profile.
Figure 4.12. Side view of $\lambda_2 = -0.01$ isosurfaces and isocurves (on $z = 24$) at $Re = 200$ for $d/D = 1.5$ (A), 2.0 (B), 3.0 (C).

to the leading sphere in accordance with the streamline profiles.

4.3.3 Pressure and Shear Distributions

Figures 4.13 and 4.14 show the pressure coefficient profile, $C_p = (p - p_\infty)/0.5\rho U^2$, over the leading and trailing spheres for $Re = 2$ and 150, respectively. At $Re = 2$ and $d/D = 6$ (plots A.2 and B.2 of Figure 4.13), both spheres present similar profiles. The maximum and minimum pressures on the bottom of the sphere shows the deviation in stagnation points caused by the presence of the wall. As $d/D$ is decreased, the pressure on the rear of the leading sphere increases, and the pressure on the front of the trailing sphere decreases. For the corresponding opposite sides, there is relatively no change. This causes a reduction in drag force experienced by both spheres. For both spheres, the pressure on the bottom is predominantly higher than on the top at large $d/D$. However, as $d/D$ is decreased, this dominance is enhanced for the leading sphere, while it is reversed for the
trailing sphere. This leads to a pressure contribution to the lift force pointing away from the wall for the former and towards the wall for the latter. The top pressure profile of the trailing sphere at \( d/D = 1.5 \) shows a maximum value at a similar angle as the bottom profile. This is part of the overall trend of the flow field in the gap region to become more symmetric at small separation distances.

Figure 4.13. Pressure coefficient profile on \( z = 24 \) for \( Re = 2 \). Rows A and B correspond to the leading and trailing spheres, respectively.

For the case of \( Re = 150 \), variations are more subtle, and the focus here is on the transition observed around \( d/D = 2 \). In the case of the leading sphere (plots A.1 and A.2 of Figure 4.14), pressure is predominantly higher on the bottom region for both separations (\( d/D = 2.3 \) and 1.8), which suggests that the pressure contribution pushes the sphere away from the wall in both cases. The opposite behavior occurs for the trailing sphere: pressure on the top region is predominantly higher, causing a lift force towards the wall at both separations shown in Figure 4.14. There are some noteworthy points to be made about the trailing sphere. Firstly, there is a delay in flow separation in its
wake, occurring at larger angles than in the case of the leading sphere and indicating an attenuation of wake effect in creating lift forces. Secondly, the highest pressures in the front of the sphere for both separations are shifted toward $\theta \approx \pi/4$; however, at $d/D = 2.3$, the pressure on top of the sphere is higher than the bottom. This change, as observed in plots B.1 and B.2, occurs between $d/D = 1.8$ and 2.0 and is related to the change from an asymmetric wake to a more symmetric one (Figure 4.8), which reflects the way the fluid approaches the trailing sphere, especially for $Re \geq 100$. Lastly, note the significant front-rear pressure drop change with $d/D$ in contrast to the negligible change experienced by the leading sphere, explaining the stronger reduction in drag for the trailing sphere (seen in next sections).

Figure 4.14. Pressure coefficient profile on $z = 24$ for $Re = 150$. Rows A and B correspond to the leading and trailing spheres, respectively.

Now we look at the contribution of shear stress to the lift forces experienced by the spheres. The following equation describes how the force in the y-direction due to viscous
effects is calculated:

\[
\frac{F_{\text{viscous}}}{\rho d^2 U^2} = \frac{1}{Re} \int \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) n_x + \left[ 2 \frac{\partial v}{\partial y} \right] n_y + \left[ \frac{\partial w}{\partial y} + \frac{\partial u}{\partial z} \right] n_z \right) dA,
\]

where \( F_{\text{viscous}} \) and \( A \) are the y-direction force due to viscous effects on the sphere and the area of the sphere; \( n = (n_x, n_y, n_z) \) is the unit vector pointing outward from the sphere surface. In this case, the z-component, \( n_z \), is zero, since only the shear profile on \( z = 24 \) is investigated. Figures 4.15 and 4.16 show \( S_x n_x + S_y n_y \), which is the shear stress in the y-direction and where \( S_x = (1/Re)(\partial u/\partial y + \partial v/\partial x) \) and \( S_y = (1/Re)(2\partial v/\partial y) \).

Figure 4.15. Shear stress profile in the y-direction on \( z = 24 \) for \( Re = 2 \). Rows A and B correspond to the leading and trailing spheres, respectively.

Both spheres present similar profiles at large distances \( d/D = 6 \). The front of the spheres has a shear stress distribution predominantly towards positive, that is, pointing away from the wall; while on the rear, it is predominantly negative. As with the pressure distribution, the reduction in \( d/D \) causes variations on the rear and front of the leading
and trailing spheres, respectively. Overall, the effect is to reduce the shear stress magnitude in these regions, which causes an enhancement of the positive lift force for the leading sphere and the induction of a negative lift force for the trailing sphere.

The case of \( Re = 150 \) is shown only for \( d/D = 1.8 \) and \( d/D = 2.3 \) (Figure 4.16). The change of shear stress magnitude between the front and back of the leading sphere is quite high, reflecting the slow moving flow field in its wake and making the variation with \( d/D \) to appear insignificant. However, effects are still present and act mainly in the rear region as in the pressure distribution profile. The profile for the trailing sphere shows a wavy behavior which is related to the four circulation regions surrounding it. The region of largest magnitude occurs right after the location, at larger angles, where the upstream flow impinges the trailing sphere. The variation with \( d/D \) occurs more significantly in the front region of the sphere. First, note the more symmetric behavior at \( d/D = 1.8 \) from \( \theta = 0 \) to \( 0.5\pi \). Then, at \( d/D = 2.3 \), the profiles are skewed toward negative values from \( \theta = 0 \) to \( 0.25\pi \) and toward positive values from \( \theta = 0.3 \) to \( 0.5\pi \).

Evidently, viscous effects are more significant at lower \( Re \). Table 4.2 shows a comparison between the average total stress in the \( y \)-direction, \( F_L/A \), and the viscous shear calculated based on the sum of the points \( S_xn_x + S_yn_y \) on \( z = 24 \). Let us take the results for the trailing spheres. At \( Re = 2 \), the relative change of \( F_L/A \) for the cases \( d/D = 1.5 \) and 3.0 is 88%; while, the relative change of the \( \sum S_xn_x + S_yn_y \) is 86%. At \( Re = 150 \), the same comparison, but for \( d/D = 1.8 \) and 2.0, leads to changes of 90% and 52% for the total and viscous stresses, respectively. Zeng and Balachandar (2005) showed a higher contribution of pressure effects on the lift force at \( Re = 150 \) for a single sphere. However, it is reasonable to see these percentages for the trailing sphere as it is exposed to a weaker flow field. They indicate that both pressure and viscous effects contribute to the variation of lift forces. If the same calculation is performed for the leading sphere at \( Re = 150 \), the results are 37% and 18% for the total and viscous stresses, respectively, showing a slightly higher contribution from the pressure effects in agreement with [112].
4.3.4 Drag Coefficient

Figure 4.17 shows the plots of the drag coefficient normalized by the single sphere drag coefficient against the separation distance \((d/D)\) between particles. Both spheres experience a reduction in drag coefficient relative to the case of a sphere in isolation. For the trailing sphere (plot B), the trend remains the same up to \(Re \approx 100\). For \(Re > 100\), the reduction of the ratio with \(Re\) diminishes for \(d/D > 3\), increasing again at smaller separations. At \(Re = 200\) and \(d/D = 1.5\), the trailing sphere experiences only approximately 25% of the single sphere drag.

Overall, the decay of the ratio with decrease in separation is more moderate for the leading particle (plot A). As opposed to the trailing sphere, the largest reduction in drag for the leading one occurs at \(Re = 2\) and \(d/D = 1.5\). At this separation, the increase in \(Re\) causes the reduction to diminish, although such behavior is not observed at every
Table 4.2. Resultant stress in the y-direction calculated based on total lift force and sphere surface area ($F_L/A$) and resultant shear stress in the y-direction based on points along circumference of sphere on plane $z = 24$.

<table>
<thead>
<tr>
<th>$d/D$</th>
<th>$Re = 2$</th>
<th>$Re = 150$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>leading sphere</td>
<td>trailing sphere</td>
</tr>
<tr>
<td></td>
<td>$F_L/A \sum S_x n_x + S_y n_y$</td>
<td>$F_L/A \sum S_x n_x + S_y n_y$</td>
</tr>
<tr>
<td>1.5</td>
<td>0.228</td>
<td>2.30</td>
</tr>
<tr>
<td>3.0</td>
<td>0.138</td>
<td>1.46</td>
</tr>
<tr>
<td>6.0</td>
<td>0.107</td>
<td>1.07</td>
</tr>
</tbody>
</table>

Figure 4.17. Normalized drag coefficient $C_D/C_{D,\text{single}}$ for leading (A) and trailing (B) spheres as a function of separation distance $d/D$ at different $Re$.

separation. Especially for the cases with $Re \geq 150$, it is possible to see a transition occurring where, as particles get closer, the drag ratio initially decreases, reaches a minimum and then increases. The place where the minimum value occurs seems to shift toward smaller values of $d/D$, with the increase in $Re$. A comparison with previous numerical results is shown in Figure 4.18.

In their case [81], the unbounded flow past two aligned spheres was studied. The comparison of our results near the wall from [81] in the bulk show more significant deviations at $Re = 200$ for the trailing sphere for all separations, with the largest deviation at $d/D = 6$. Similarly, for the leading particle, deviations with respect to the unbounded
Figure 4.18. Comparison between present study with spheres near the wall and results of [81] in the bulk for $C_D/C_{D,\text{single}}$ of leading (A) and trailing (B) spheres as a function of separation distance $d/D$ at different $Re$.

case become more relevant at $Re = 200$, although only for $d/D < 3$. It is interesting to note that in both cases, near the wall or in the bulk, the drag coefficient for the leading sphere undergoes the transition described above, in this case, at about $d/D = 3$ for $Re = 200$. This was explained in [81] as the result of the trailing sphere interfering with the wake of the leading one. As also mentioned in their work, the increase in $Re$ induces a larger wake length, which explains why the transition occurs at larger separations for larger $Re$. With this comparison, it is possible to say that the presence of the wall has a negligible effect on the hydrodynamic interaction that contributes to the drag experienced by two aligned spheres at least for $L/D \geq 1$ and $50 \leq Re \leq 200$. This is interesting especially because in the case of the bounded flow at $Re = 200$, the leading sphere produces an asymmetric wake with double-thread structure at $d/D = 3$. The latter is suppressed at $d/D = 2$ and the former at $d/D = 1.5$. These changes have virtually no effect on the profile of the leading sphere drag coefficient ratio. Additionally, the presence of the wall and its effects to the wake of the leading sphere has merely a quantitative influence to the drag experienced by the trailing sphere, with relatively more significant deviations only at $Re = 200$.

Figure 4.19 shows the change with respect to $Re$ at different $d/D$ for the trailing sphere. The general trend for the decay of the drag coefficient ratio with $Re$ may be described by a simple power law, $ARe^B$. Specifically at $d/D = 3$, the decay is very well captured by the expression: $0.93Re^{-0.12}$, with a coefficient of determination, $R^2 =$
0.995, and 95% confidence bounds of (0.90 and 0.96) and (-0.11 and -0.13) for A and B, respectively.

Figure 4.19. $C_D/C_{D,\text{single}}$ for trailing sphere as a function of $Re$ at different $d/D$.

Deviations from such expression arise as $d/D$ is changed, but a clear and significant transition emerges at lower $d/D$. In this case, deviations initiate at higher $Re$, such that at $d/D = 1.5$, a transition of scaling seems to occur at $Re = 50$. This indicates a qualitative change in the hydrodynamic interaction between spheres occurring within this close region of $d/D = 3$.

4.3.5 Lift Coefficient

Figure 4.20 and 4.21 show the variation of the lift coefficient ($C_L/C_{L,\text{single}}$) ratio against $d/D$ at different $Re$. Especially at $Re = 2$, a considerable increase in lift coefficient is observed (Figure 4.20) for the leading sphere, reaching at $d/D = 1.5$ a value more than twice as much that experienced in the single-sphere condition. Such behavior is mainly related to the change in shear stress profile in the rear of the leading sphere due to the flow separation induced by the trailing sphere. The increase of lift coefficient ratio with lower $d/D$ diminishes with the increase in $Re$ until $Re \approx 100$. Then, for $Re \geq 150$, the trend starts to present a local maximum value at $d/D = 2$. While the local minimum in drag coefficient ratio (plot A of Figure 4.17) had little to do with the presence of the wall, the behavior observed here only appears because of the wall. Such behavior can be well correlated with the observed flow field patterns for $Re > 150$. Initially, at $d/D = 4$ and 3, the trailing sphere has some impact on the wake of the leading one, but overall the topology of the wake remains the same. It is only at $d/D \approx 2$ that the leading sphere
Figure 4.20. Normalized lift coefficient $C_L/\text{C}_\text{L,single}$ for leading sphere as a function of separation distance $d/D$ at different $Re$.

The wake undergoes a significant change. The asymmetry is magnified by the suppression of the bottom circulation region at $d/D = 2$, which is related to the increase in lift coefficient ratio. With further decrease in separation, a more symmetric structure appears in the wake of the leading sphere, causing the drop observed in Figure 4.20. At $Re = 200$ and $d/D = 1.5$, the lift coefficient of the leading sphere is half of the single-sphere case value.

The trailing sphere experiences stronger variations as a function of $d/D$. Figure 4.21 shows two different trends for cases with $2 \leq Re < 50$ (plot A) and $50 < Re < 200$ (plot B). Even at large separations, $d/D > 4$, and low $Re$, the lift coefficient of the trailing sphere suffers significant reduction. Plot (A) shows that a reversal in the direction of lift force occurs as $d/D$ is decreased, which is accentuated at lower $Re$. At $Re = 2$ and $d/D = 1.5$, the trailing sphere experiences the opposite lift force as that encountered in a single-sphere situation. These variations of the translation-induced lift forces at low $Re$ for both spheres demonstrate the destabilizing effect of inter-particle hydrodynamic interactions on the lateral and axial alignment of particles in microfluidic devices [67].

At $Re = 50$, the drop in lift force is attenuated, and the value seems to be reaching zero as spheres approach each other. In plot (B), we see a shift in the trend as $Re$ increases. The drop in lift coefficient ratio starts to accentuate again with the decrease in $d/D$ up to $d/D = 2$, when the ratio shoots back up. Both the reversal and the transition are observed in Table 4.2, that is, the shear stress in the vertical direction ($S_xn_x + S_yn_y$) on the $z = 24$ plane captures these variations. The asymmetric wake produced by the
leading sphere gains increasingly more importance on the lift forces experienced by the trailing one for \( Re > 50 \). This can be visualized by how the flow field impinges on the trailing sphere (Figure 4.8) and by the increased strength of the top vortical structure at \( d/D = 2 \) (Figure 4.10). The importance of the type of wake is also demonstrated by the magnitude decrease observed at \( d/D = 1.5 \). The transition into a more symmetric flow pattern in the wake of the leading sphere induces a smaller lift force.

It is also worth noting the variation of lift coefficient with \( Re \) at different \( d/D \). As observed in Figure 4.22, the largest deviations for the leading sphere occur at low and high \( Re \) conditions, particularly at small separations. As reported before [112], a single sphere experiences an increased lift force as the asymmetry of the wake flow is enhanced with the increase in \( Re \), past approximately 100. Such behavior is abruptly suppressed as spheres approach each other (\( d/D = 2 \) to 1.5), going from an enhanced increase in lift to a dampened one, where the lift continues to decrease with \( Re \). At the other extreme, \( Re < 10 \), the curves for the leading particle deviate from the single-sphere case as \( Re \) decreases, with larger deviations at lower \( d/D \).

Figure 4.23 shows significant changes of the lift force for the trailing sphere compared to single-sphere case. As observed in plot (B), the increase in lift for a single sphere past \( Re = 100 \) is increasingly suppressed with lower \( d/D \). While this is caused by a change in the wake pattern and happens abruptly for the leading sphere, the deviation observed
Figure 4.22. $C_L/C_{L,single}$ for leading sphere as a function of separation distance $Re$ at different $d/D$ for the trailing sphere is caused by the approaching flow field and is significant even at $d/D = 6$.

Figure 4.23. $C_L/C_{L,single}$ for trailing sphere as a function of separation distance $Re$ at different $d/D$

Larger deviations from the single-sphere trend, and reversal of lift direction, starts first at higher $Re$ due to larger leading-sphere wakes. The points not shown in plot (B) are negative, so for the case of $d/D = 2$, the sphere experiences an attractive force towards the wall for all $Re$. In plot (A), it is observable that the strength of the reversal in lift direction is relatively much more significant at lower $Re$. Such behavior of wall-directed lift forces is expected to play a significant role in the dispersion characteristics of particle-laden flows nearby a wall, particularly in the case of sedimentation of dilute particle systems. A preliminary indication of this is given by the study of Uhlmann and
Doychev (2014), where they report the tendency of particles to align vertically in their fully-periodic simulations of sedimentation of dilute systems. Further, investigation is necessary to attest this.

4.4 Conclusion

In this work, a newly implemented code, combining the DLM/FD methodology with the open source Basilisk framework, was utilized for the study of the effects of stationary walls on the hydrodynamic interactions between nearby spheres. The implementation was validated against results of drag and lift coefficients as well as pressure distributions obtained from previous studies on wall-induced forces on a single sphere using spectral element method. A two-sphere system in tandem arrangement was investigated where the separation distance between spheres was varied while the distance between the wall and spheres was kept constant. The presence of the wall induces asymmetry of the flow field surrounding the spheres, which undergoes significant transitions as the separation distance \((d/D)\) is varied. Consequently, the hydrodynamic forces experienced by the spheres are modulated. In this regard, the key findings are summarized as follows:

- At least for \(L/D \geq 1\) and \(50 \leq Re < 200\), the presence of the wall has negligible effects on the hydrodynamic interactions that contribute to the drag experienced by two aligned spheres. This is especially significant accounting for the flow structure transitions that occur. For example, a double-thread structure is suppressed within \(1.5 \leq d/D \leq 3\) at \(Re = 200\). Nevertheless, the drag coefficient ratios of both spheres follow the same qualitative trend as the case in unbounded flows.

- The lift forces acting on both spheres are more sensitive to the variations in flow field associated with separation distance:
  - At low \(Re\), the leading sphere experience significant increase of lift force pointing away from the wall; while, the trailing sphere experiences a reversal in lift force direction.
  - At high \(Re\), both spheres undergo a transition which ultimately leads to a reduction in lift magnitude. The lift forces of the leading and trailing spheres
go through a maximum and minimum, respectively. These transitions are linked to the variations in flow structures in the wake of the leading sphere: (1) increasingly stronger vortical structures in the upper half of the wake with $Re$ and (2) suppression of the asymmetry with separation distances, $d/D$, below 2.
Chapter 5. Summary and Future Recommendations

Both developed and incipient codes were utilized in this work to investigate different scenarios of particle-laden flows. The CFD-DEM approach was applied to the study of highly dense pulsed fluidized beds, where a large number of particles were simulated (400,000 - 800,000). It was qualitatively demonstrated that the implemented models contain the correct physics for the reproduction of the experimentally obtained staggered pattern behavior. In a more in-depth analysis, the effects of pulsation parameters - mean flow rate ($V_M$) and amplitude of oscillation ($V_A$) - were assessed, revealing a transition in the particle bed behavior as $V_A$ is varied while keeping $V_M$ constant. In particular, the average coordination number of the particle bed was able to capture such transition, showing that a stronger suppression of the incoming void layers resulted in a change in the dynamics of the bed. This has important practical implications. For example, as shown in Chapter 2, it is possible to adjust pulsation parameters to attain optimized conditions of gas-solid interaction, being it at lower or higher coordination number. We expect the results to motivate further computational and experimental investigation of the parametric space and fine-tuning of pulsation parameters.

The Basilisk-DLM/FD code was applied to perform a high-resolution investigation of the effects of a wall on the hydrodynamic of two nearby spheres. This is representative of a more dilute system. In this work, we investigated the hydrodynamic interactions of two spheres in tandem arrangement in a range of flow conditions $2 \leq Re \leq 200$ and separation distances ($1.5 \leq d/D \leq 6$), under the influence of a wall. The variation in hydrodynamic forces was correlated to changes in flow field as $d/D$ was varied. As in previous studies, the presence of the wall induced the appearance of flow structures at earlier flow conditions ($Re$) in comparison to unbounded cases. An interesting phenomenon is the suppression of the asymmetric behavior at $d/D < 2$, which induces a reduction in lift force magnitude. A key finding of this study was that even with significant flow structure changes with $d/D$ variation, such as suppression of double-thread structures and asymmetric flow field, the proximity to the wall had a negligible effect on the hydrodynamic factors that contribute to the drag force experienced by the spheres. These insights are of relevance to the
development of large-scale models. Evidently, the studies presented here require more investigation and can be readily advanced by further exploration of the parametric space.

A broader contribution of this work was the investigation of the limitations and qualities of the codes, applying them to unexplored conditions of particle-laden flows. In this regard, we also provide preliminary verification and validation cases in Appendix A, which can point in the direction of future investigations. A recently implemented Gaussian-weighted average for the computation of void fraction in the CFD-DEM code was tested, and the capabilities of the Basilisk-DLMFD-Grains3D implementation for direct numerical simulation of moving particles was assessed. The evolution of cluster of particles settling in a viscous fluid is an example of a topic that can take advantage of the mentioned capabilities. Some small scale systems, such as the experimentally investigated in [76] and [22], can be used as basis for direct comparison between CFD-DEM and PR-DNS; this type of system allow for the identification of pitfalls of the CFD-DEM approach and quantification of hydrodynamic interactions between particles, using PR-DNS.
Appendix A. Verification and Validation Cases

A.1 CFD-DEM

A.1.1 Introduction

The CFD-DEM code used in this Work is at an advanced stage of development. It has been used in a variety of physical scenarios involving particulate matter, such as fluidization, Rayleigh-Taylor instability, rotating tumblers and shaker tables [104, 111, 6, 74, 110], demonstrating its level of robustness. Nevertheless, continuing improvement is performed for the advancement of its scope of applicability. One such advancement is considered in this section.

A fundamental assumption in the development of the volume-averaged equations used in CFD-DEM approaches is that the averaging length scale ($l_{avg}$), which is represented by the CFD cell size ($\Delta x$), is much larger than the solid-phase length scale ($d_p$) and much smaller than the largest scales in the system (e.g. equipment size, $L$). In the fluid momentum and continuity equations, the presence of the solid phase is partly manifested through its volume fraction, which classically has relied on the fact that $\Delta x >> d_p$ for its correct calculation. This poses a significant limitation to the use of CFD-DEM for cases where $L \approx 10 - 100d_p$, and has practical implications as well. Let us take the example of sand retention procedures in the exploration of hydrocarbons. Stand-alone screens are one of the simplest methodologies used for this purpose. As the name suggests, the main barrier impeding the sand from traveling through the base pipe up to surface facilities is a screen. There is great variability in the sand released from the rock formation with regards to its polidispersity characteristics, and this makes the choice of screen gap sizes to be a challenging task. Once chosen, the screen gap becomes a major factor dictating the fluid length scales near the screen as a converging flow arises there [15]. Evidently, this gap is also larger than a portion of the sand sizes, thus creating a conflict for classical CFD-DEM approaches: a fine grid is required near the gap but cells must be larger than the largest particles for the correct volume fraction computation. Due to conflicts such as this one, many studies have come up with new ways for uncoupling the CFD cell size from the particle volume fraction calculation. Capecelatro and Desjardin (2013) have
proposed a two-step filtering process. First, the Lagrangian data associated with the particles are transferred to the Eulerian frame by a Gaussian-weighted average. Let us take for example the particle volume fraction computation:

\[ \phi = \sum_{i=1}^{N_p} w(r) V_{p,i}, \quad w(r) = \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{r^2}{2\sigma^2}} \]  

(A.1)

where \( r \) and \( V_{p,i} \) are the particle-to-cell distance and particle volume, respectively. By choosing a kernel width (or standard deviation), \( \sigma = \Delta x / 2\sqrt{2\ln 2} \), the full width at half maximum of the distribution becomes \( \Delta x \) and the effect of a particle is spread out over the 27 nearest cells. This first step already enables \( \Delta x \approx d_p \) to be used in the CFD-DEM approach. However, for cases with finer mesh, a second step is necessary. In this case, the Eulerian field created in the previous step is diffused such that the distribution of the particle properties on the Eulerian frame attains a characteristic length scale that fulfills the aforementioned assumption. As this step is not performed here, we direct the reader to the cited work for a more detailed description. Additionally, for another approach, the reader is directed to [63].

Recently, the DEM code used in this work was upgraded to include a Gaussian-weighted average approach for the Lagrangian-Eulerian data transfer. Earlier, the code relied only on analytical expressions to calculate the particle volume contained by a given cell, which ultimately lead to an accurate computation of the particle volume fraction field. However, this limited the code to the use of cells that were sufficiently large to encompass at least a few particles. In this work, we provide some preliminary validation of the most recent version of the DEM code.

A.1.2 Problem Description

Simulations of pseudo-2D fluidized beds were performed for cases with experimental equivalents. Two previous experimental studies were chosen to test our numerical methodology. The first consisted of a fluidized bed made of polystyrene particles from which pressure, voidage and bed height measurements were obtained [94]. The second system consisted of poppy seeds from which Magnetic Resonance (MR) measurements were
Figure A.1. A representative snapshot of the 3D particle bed.

captured and translated into average velocity, bubble granular temperature and voidage profiles along the bed [71, 72]. Figure A.1 is a depiction of the type of systems studied in this work, which also serves as reference for other chapters. Note the 3D character of the particle bed system.

Table A.1 shows the CFD-DEM parameters for the base case used to reproduce the results presented in the aforementioned studies. Additionally, It is important to point out that the Beetstra drag correlation was used in this case [7].

Table A.1. Parameters of CFD-DEM base case simulations of Muller et al. 2008 and 2009 (Muller) and van Wachem et al. 2001 (Wachem).

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value (Muller)</th>
<th>Value (Wachem)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Solid phase</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Particle diameter ($d_p$ mm)</td>
<td>1.2</td>
<td>1.28</td>
</tr>
<tr>
<td>Particle density ($\rho_p$ kg/m$^3$)</td>
<td>1000</td>
<td>1150</td>
</tr>
<tr>
<td>Restitution coefficient ($e$)</td>
<td>0.98</td>
<td>0.9</td>
</tr>
<tr>
<td>Poisson ratio ($\nu$)</td>
<td>0.33</td>
<td>0.25</td>
</tr>
<tr>
<td>Friction coefficient p-p ($\mu_C$)</td>
<td>0.1</td>
<td>0.3</td>
</tr>
<tr>
<td>Friction coeff. lateral walls ($\mu_{C,W}$)</td>
<td>0.0</td>
<td>0.3</td>
</tr>
<tr>
<td>Young’s modulus ($E$ MPa)</td>
<td>0.12</td>
<td>100</td>
</tr>
<tr>
<td><strong>Fluid phase</strong></td>
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<td></td>
</tr>
<tr>
<td>Fluid density ($\rho_f$ kg/m$^3$)</td>
<td>1.225</td>
<td>1.28</td>
</tr>
<tr>
<td>Fluid viscosity ($\mu$ Pa · s)</td>
<td>$1.8 \cdot 10^{-5}$</td>
<td>$1.7 \cdot 10^{-5}$</td>
</tr>
<tr>
<td><strong>Geometry, Mesh, Time step</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Bed ($W \times H \times T$ mm$^3$)</td>
<td>44 x 288 x 10</td>
<td>90 x 450 x 8</td>
</tr>
<tr>
<td>Cells ($N_u \times N_y \times N_z$)</td>
<td>24 x 160 x 1</td>
<td>10-40 x 50-200 x 1</td>
</tr>
<tr>
<td>Fluid time step</td>
<td>$1 \cdot 10^{-4}$</td>
<td>$1 \cdot 10^{-4}$</td>
</tr>
<tr>
<td>DEM time step</td>
<td>$2 \cdot 10^{-6}$</td>
<td>$2 \cdot 10^{-6}$</td>
</tr>
</tbody>
</table>
A.1.3 Results and Discussion

Figure A.2 shows the qualitative features of the fluidization occurring in both systems mentioned above, even though it is extracted from the simulations related to the van Wachem et al. (2001) case. It is possible to observe a slugging behavior, where void structures grow to become as large as the lateral domain size. The emergence, growth and eruption of these structures occur in a periodical fashion and are represented by a dominant frequency of oscillation, which can be assess by pressure measurements.

In their work [94], the authors report the power spectrum distribution (PSD) of the pressure oscillation collected from a height of 45mm, showing a primary peak at approximately 2.4Hz. In Figure A.3, we show the effect of refining the mesh size on the dynamic behavior of our simulation. This is done such that the Gauss-weighted average, as discussed in the Introduction, is used for the case where \( \Delta x/d_p = 1.5 \). The mesh is not
refined along the depth of the bed, and 1 fluid cell in this direction is kept for all cases as the phenomena occurring in pseudo-2D beds are most sensitive to the resolution in the other two dimensions [71, 105]. Observe that the main frequency of oscillation decreases, toward the experimental value, as the mesh is refined, or $\Delta x/d_p$ is decreased. Note also the very good agreement with regards to the power-law decay slope for $\Delta x \leq 3d_p$.

The deviation in intensity of PSD between our results and experimental data, observed in Figure A.3, is due to the different ways in which the PSD is scaled. This can be attested by a comparison in relative pressure time series. The standard deviation calculated based on the observed time frame (Figure A.3) is 83.2 and 83.9 for experimental and simulation results, respectively. We want to point out that in [94], the authors provide only a section of the total time series, but their PSD is based on the complete time series. In our case, the PSD is calculated based on a time span of 7 seconds (3 - 10s) with a sampling frequency of 10000Hz.

The decrease in frequency of oscillation is also readily observed in the bed height time series (Figure A.4). Note also the increase in maximum heights attained by the particle bed. This has to do with a significant inflation of the slugs as they reach the surface of the bed with decreasing $\Delta x/d_p$. Additionally, at $\Delta x/d_p = 6$, the bubble roof mainly "rains down" as the void structure travels up the bed, contrary to the frequent splitting phenomenon occurring at lower $\Delta x/d_p$, observed in the simulation videos. This suggests
Figure A.4. Experimental and numerical bed height time series.

a better resolution of the Rayleigh-Taylor instability present in solid-fluid systems [111]. Table A.2 shows the mean and standard deviations for the bed height. Both of these increase towards the experimental values.

Table A.2. Bed height statistical quantities (average ± standard deviation).

<table>
<thead>
<tr>
<th>∆x/d_p</th>
<th>0.107±0.004</th>
<th>0.112±0.009</th>
<th>0.116±0.012</th>
<th>0.120±0.019</th>
</tr>
</thead>
</table>

This larger expansion at the surface seems to delay the emergence of subsequent slugs, causing only smaller void structures to appear, which can be seen in the average particle volume fraction time series, collected from 45mm (Figure A.5). As observed, bubble passage is very regular in the case of ∆x/d_p = 6; while, such behavior is disrupted with decreasing ∆x/d_p. This is in agreement to the referred delay in forming large slugs and the increase in the splitting phenomenon. Based on the limited time span provided by the authors [94], overall, the simulation results show a more compact system than the experimental one, with higher maximum and minimum average particle volume fraction.

Next we provide another set of comparisons based on the experimental data in [71, 72]. Again, we use the Gaussian-weighted average for the computation of void fraction, and the parameters used in this case are described in Table A.1. These experimental references were chosen for composing a small size system, consisting of 9240 particles, and for providing a variety of measurements. Additionally, the reported experimental data has been extensively used by the community as validation basis for CFD-DEM.
Figure A.5. Experimental and numerical particle volume fraction time series.

approaches [59, 33, 75, 31]; thus, allowing for verification of our results. Such verification may be observed in Figure A.6, where the average axial velocity at different heights in the bed are plotted with other numerical studies. Overall, deviations of our results from experiments are within the range observed in other numerical studies. Specifically, our results generate smaller velocity magnitudes both at the center and sides of the bed, matching better the results obtained by Peng et al. (2014) , who used the MFIX-DEM code developed at National Energy Technology Laboratory. With respect to the experimental results, larger deviations are overall observed in the middle of the bed where the effect of passing bubbles is more pronounced. Next we show a sensitivity analysis with respect to the dissipative character of the system by varying the friction coefficient. Figure A.7 shows the effect of this parameter on the average bubble granular temperature and voidage at two different heights in the bed.

Overall, the fluctuations of particle velocity, described by bubble granular temperature, is higher in the middle of the bed, as expected. This is where the effect of bubbles is concentrated. However, simulations generate bubbles that have a wider extension, causing
Figure A.6. Comparison between experimental and numerical average axial velocity at different heights in the fluidized bed.

the time-averaged voidage to be higher than the experiments near the sidewalls. Poppy seeds were used in the experiments as they can be well imaged by MR, but unfortunately their mechanical properties were not reported in [71, 72]. Their kidney-like shape and size are at the center of such deviations. This geometry might lead to inter-locking of particles near the sidewalls, causing stronger resistance for motion in these regions and ultimately affecting the whole system. Gupta et al. (2016) hinted in that direction by using side-walls consisting of fixed particles. With this approach, they reached better agreement for both axial velocity and granular temperature, but there was no comparison for voidage profiles. In Figure A.7, a more dissipative system leads to higher voidage in the middle of the bed for both heights and lower at the sidewalls at $y = 31.2 \text{mm}$, indicating such effect and approximating the simulation results both qualitative and quantitative to the experimental ones. Although, a relative small variation occurs in this case, it translates to a significant increase in bubble granular temperature, with more pronounced variation along the x-direction. This trend is in agreement with previous studies [33, 75]. However, a simple variation of dissipative characteristics is not able to fully capture the complete
Figure A.7. Bubble granular temperature (top row) and voidage (bottom row) profiles at different height in the bed of fluidized bed.
nuances of this problem. Other factors have previously been investigated. Non-sphericity was partially accounted for in the drag law by a shape factor, leading to slightly higher voidages in the middle of the bed [59], and polydispersity effects were assessed in [31] by varying the mean particle size: a change of 18% in diameter led to as much as 50% change in velocity magnitude. The exact shape of the particles and even a neglected polydispersity might be the cause for the more discrepant results at higher positions, which will not only affect particle-particle but also fluid-particle interactions. Although more precise modeling of these factors still need to be performed, it is shown here however that a simplified spherical system gives sensible results that could clarify the behavior in fluidized beds.

A.2 PR-DNS

In this section, we provide some verification cases of the Basilisk-DLM/FD-Grains3D implementation for systems with moving, interacting particles. The simplest possible scenarios are associated with the evolution of two spheres in side-by-side and aligned configurations. The latter condition is related to the well-known drafting-kissing-tumbling (DKT) phenomenon; while, the former is less known, but also extensively used as a validation case. A sketch of the configurations is shown in Figure A.8, and the base case parameters used in this section are described in Table A.3.

As mechanical interaction occurs in the case of the DKT phenomenon, the DEM
Table A.3. Parameters associated with the PR-DNS simulations against the results from Cao et al. 2015 (Cao) and Maitri et al. 2018 (Maitri).

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value (Cao)</th>
<th>Value (Maitri)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$L_x/D = L_y/D$</td>
<td>45</td>
<td>24</td>
</tr>
<tr>
<td>$S/D$</td>
<td>1.5</td>
<td>2.0</td>
</tr>
<tr>
<td>$T/D$</td>
<td>8</td>
<td>3.0</td>
</tr>
<tr>
<td>Domain size ($cm$)</td>
<td>7.5</td>
<td>4</td>
</tr>
<tr>
<td>Particle diameter ($D - cm$)</td>
<td>1/6</td>
<td>1/6</td>
</tr>
<tr>
<td>Particle density ($\rho_p - kg/m^3$)</td>
<td>1140</td>
<td>1140</td>
</tr>
<tr>
<td>Fluid density ($\rho_f - kg/m^3$)</td>
<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>Fluid viscosity ($\mu - Pa \cdot s$)</td>
<td>$10^{-3}$</td>
<td>$10^{-3}$</td>
</tr>
<tr>
<td>Terminal velocity ($U_c - m/s$)</td>
<td>0.0509</td>
<td>0.0509</td>
</tr>
<tr>
<td>Characteristic time ($T_c - s$)</td>
<td>$D/U_c$</td>
<td>$D/U_c$</td>
</tr>
<tr>
<td>Time step ($\Delta t_f - s$)</td>
<td>$T_c/50$</td>
<td>$T_c/200$</td>
</tr>
<tr>
<td>Basilisk tolerance criterion ($TOL$)</td>
<td>0.001</td>
<td>0.001</td>
</tr>
<tr>
<td>Maximum level of resolution ($ML$)</td>
<td>11</td>
<td>9</td>
</tr>
<tr>
<td>Velocity criterion threshold ($VC$)</td>
<td>0.01</td>
<td>0.001</td>
</tr>
</tbody>
</table>

Table A.4. Contact parameters of linear-spring model used in the simulation of the DKT phenomenon.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stiffness coefficient ($k_n$)</td>
<td>$8.9 \cdot 10^2$</td>
</tr>
<tr>
<td>Damping coefficient ($\eta_n$)</td>
<td>$8.5 \cdot 10^2$</td>
</tr>
<tr>
<td>Restitution coefficient ($e_n$)</td>
<td>0.9</td>
</tr>
<tr>
<td>Friction coefficient ($\mu_C$)</td>
<td>0.3</td>
</tr>
<tr>
<td>Maximum overlap ratio ($\delta_{max}/D$)</td>
<td>0.225%</td>
</tr>
<tr>
<td>DEM time step ($\Delta t_{DEM} - s$)</td>
<td>$\Delta t_f/25$</td>
</tr>
</tbody>
</table>

module Grains3D was used to simulate the contact between particles. A linear-spring formulation is used, and the guidelines described in [97] were adopted to compute the spring and damping coefficients. Table A.4 lists all the parameters associated with the collision dynamics.

Figure A.9 shows a comparison between our results and a previous numerical work [13] as well as sensitivity analysis of numerical parameters. The authors investigated and mapped the interactions of two moving spheres starting from all possible configurations, using the Lattice-Boltzmann numerical approach. In Figure A.9, we see their results for one of the spheres. Plot (A) shows the motion of a sphere in space as it settles ($y-axis$), along the direction of horizontal alignment ($x-axis$) between the spheres. The overall trend consists of a separation of the spheres at different slopes as time progresses, although they move toward each other very briefly during the beginning of the phenomenon. Plot (B) shows the respective variation of the $x$-component of velocity ($V_x$) with time. While
Figure A.9. Comparison of numerical results for the motion of a single sphere as a result of hydrodynamic repelling interactions with a second sphere (A) and respective velocity time history along the x-direction (B). Additionally, sensitivity analysis with respect to numerical parameters is shown.
Figure A.10. Comparison of the DKT phenomenon with previous numerical results of Maitri et al. 2018 ($T_c = \sqrt{D_p/g}$, $V_c = \sqrt{D_p g}$).

our base case generates quite satisfactory results for the motion in space, we see some spurious oscillation of $V_x/U_c$ starting at $t/T_c = 20$. The second row in Figure ?? shows the effect of some numerical parameters with respect to the base case. It is possible to see that a decrease in the base-case velocity criterion threshold ($V_C$) induces a significant change in the $V_x/U_c$ profile, removing the aforementioned oscillations. Additionally, the effect of different $V_C$ values is presented, with $V_C/10$ (i.e. a decade less of the base-case value) being the point at which this spurious behavior stops. When spheres are close to each other, their combined wake causes the refined mesh to extend farther away from them, capturing well the effects of the wake and surrounding area. At a certain distance from each other, the mesh becomes concentrated on the sphere, which might leave some relevant regions without appropriate resolution, causing issues such as the one described. Decreasing the value of $V_C$ has a broader effect, the whole mesh is possibly refined; whereas, changing the maximum level of resolution ($ML$) has a more local effect, especially around the spheres.

Figure A.10 shows a comparison between our results and previous numerical work [66] for a case of two vertically-aligned spheres along the $y$ direction. In their work, the authors used a variation of the immersed boundary method. The dimensionless height ($y/D_p$) and vertical velocity of the spheres ($V_p/V_c$) are plotted in Figure A.10. The DKT phenomenon is clearly seen in the $V_p/V_c$ profile. Initially, both spheres accelerate and travel downwards with same velocity. Acceleration becomes stronger for the trailing sphere as it enters the leading sphere wake (drafting), causing a contact between them (kissing). The spheres
exchange momentum, and the trailing one tumbles over the leading sphere, which can be seen in the $y/D_p$ plot near $t/T_c = 45$. In their case [66], the authors used a resolution equivalent to 56 cells over the particle diameter ($D/56$); while we used $D/21$, and we see a very good agreement between the results, although our spheres travel at a slightly higher velocity. Also, the earlier collision observed in their case may attributed to differences in the spheres lateral starting position and the lubrication model that they use to capture sub-grid phenomenon, which is activated before spheres actually contact each other.
Appendix B. Permission License

Bibliography


Hong-Wei Li and Hao Guo. “Analysis of drying characteristics in mixed pulsed rectangle fluidized beds”. In: *Powder Technology* 308 (2017), pp. 451–460.


Vita

Daniel de Oliveira was born in 1991 in Fortaleza, Brazil. He started his studies in Chemical Engineering in 2009, when he joined Federal University of Ceara. In 2012, he was financed by the Brazil Science Without Borders (BSWB) program to participate in an exchange program at University of Kentucky, where he took classes and performed research. This experience motivated him to further his studies, and after returning to Fortaleza, he obtained his bachelor’s degree in the Spring of 2014 and a 4-year doctorate scholarship under the BSWG program. He then joined Dr. Krishnaswamy Nandakumar’s group at Louisiana State University to pursue a PhD in Chemical Engineering in the Fall of 2014.