Suspensions of finite-size rigid spheres in different flow cases

by

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November 2015
Technical Reports
Royal Institute of Technology
Department of Mechanics
SE-100 44 Stockholm, Sweden
Akademisk avhandling som med tillstånd av Kungliga Tekniska Högskolan i Stockholm framlägges till offentlig granskning för avläggande av teknologie licentiatsexamen torsdag den 17 december 2015 kl 14.00 i sal D3, Kungliga Tekniska Högskolan, Lindstedtvägen 5, Stockholm.

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“Considerate la vostra semenza:
fatti non foste a viver come bruti,
ma per seguir virtute e canoscenza”

Dante Alighieri, Divina Commedia, Inferno, Canto XXVI
Suspensions of finite-size rigid spheres in different flow cases

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Abstract

Dispersed multiphase flows occur in many biological, engineering and geo-
physical applications such as fluidized beds, soot particle dispersion and pyro-
clastic flows. Understanding the behavior of suspensions is a very difficult task. Indeed particles may differ in size, shape, density and stiffness, their concentration varies from one case to another, and the carrier fluid may be quiescent or turbulent. When turbulent flows are considered, the problem is further com-
plicated due to the interactions between particles and eddies of different size, ranging from the smallest dissipative scales up to the largest integral scales. Most of the investigations on the topic have dealt with heavy small particles (typically smaller than the dissipative scale) and in the dilute regime. Less is known regarding the behavior of suspensions of finite-size particles (particles that are larger than the smallest lengthscales of the fluid phase).

In the present work, we numerically study the behavior of suspensions of finite-
size rigid spheres in different flows. In particular, we perform Direct Numerical
Simulations using an Immersed Boundary Method to account for the solid phase. Firstly is investigated the sedimentation of particles slightly larger than the Taylor microscale in sustained homogeneous isotropic turbulence and quiescent fluid. The results show that the mean settling velocity is lower in an already turbulent flow than in a quiescent fluid. By estimating the mean drag acting on the particles, we find that non stationary effects explain the increased reduction in mean settling velocity in turbulent environments.

We also consider a turbulent channel flow seeded with finite-size spheres. We change the solid volume fraction and solid to fluid density ratio in an idealized scenario where gravity is neglected. The aim is to independently understand the effects of these parameters on both fluid and solid phases statistics. It is found that the statistics are substantially altered by changes in volume fraction, while the main effect of increasing the density ratio is a shear-induced migration toward the centerline. However, at very high density ratios (∼ 100) the two phases decouple and the particles behave as a dense gas.

Finally we study the rheology of confined dense suspensions of spheres in simple shear flow. We focus on the weakly inertial regime and show that the suspension effective viscosity varies non-monotonically with increasing confinement. The minima of the effective viscosity occur when the channel width is approximately an integer number of particle diameters. At these confinements, the particles self-organize into two-dimensional frozen layers that slide onto each other.
Descriptors: particle suspensions, sedimentation, homogeneous isotropic turbulence, turbulent channel flow, rheology.
Suspensioner av stora stela sfärer i olika flödesfall

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Sammanfattning
I många biologiska, tekniska och geofysiska tillämpningar förekommer flerafasströmning. Fluidiserade bäddar, fördelning av sotpartiklar och pyroklastiska flöden är några exempel på sådana tillämpningar. Att förstå partikelsuspensioner och dess egenskaper är en svår uppgift. Partiklarna kan variera i storlek, form, densitet och styvhet, partikelkonzentrationen kan variera från fall till fall, och den transporterande vätskan kan vara stilla, men även turbulent.


I detta arbete studeras beteendet hos suspensioner bestående av stela sfärer (större än de minsta turbulenta virvlar) för olika strömningsfall med hjälp av Direkt numerisk simulering (DNS). I simuleringarna hanteras partikelfasen (soliden) med hjälp av en såkallad Immersed Boundary metod. Först undersöker vi sedimentationen hos partiklar som är något större än Taylors mikroskala i upprätthålLEN homogen isotropisk turbulens samt i en stilla fluid. Resultaten visar att den genomsnittliga sedimenteringshastigheten är lägre i en redan turbulent strömning jämfört den i en stilla fluid. Genom att uppskatta det genomsnittliga motståndet på partiklarna, finner vi att icke-stationära effekter förklarar den ökade minskningen i genomsnittliga sedimenteringshastigheten som återfinns i turbulenta miljöer.

Turbulent kanalströmning innehållande sfäriska partiklar studeras också inom ramen för detta arbete. Partikelns volymfraktion varierar samt densitet förhållandet partikel och vätska då strömningen är sådan att gravitationen kan försummas. Målet är att förstå hur de oberoende effekterna av ovanstående parametrar påverkar de statistiska egenskaperna hos både vätske- och partikelfasen. Resultaten visar att de statistiska egenskaperna förändras avsevärt då volymfraktionen ändras medan den huvudsakliga effekten av förändring i densitetsförhållandet är en skjuvinducerad förflyttning av partiklarna mot centrumlinjen. Vid väldigt höga densitetsförhållanden (~ 100) separeras emellertid de två faserna åt och partiklarna beter sig som en tät gas.

Slutligen studerar vi relogin hos avgränsade suspensioner med hög partikelkonzentrationen av sfärer i en enkel skjuvströmning. Vi fokuserar på den svagt
tröga regimen och visar att suspensionens effektiva viskositet varierar icke-monotont med ökad avgränsninggrad. Den effektiva viskositeten uppvisar ett minsta värde då kanalens bredd är approximativt en multipel av partikeldiameter. Vid dessa avgränsningar där avståndet mellan två väggar minskas mer och mer så ordnar sig partiklarna i tvådimensionella lager som glider ovanpå varandra.

Deskriptorer: partikelsuspensioner, sedimentering, homogen isotropisk turbulens, turbulent kanalströmning, reologi.
Preface

This thesis deals with the study of the behavior of suspensions of finite-size particles in different flow cases. An introduction on the main ideas and objectives, as well as on the tools employed and the current knowledge on the topic is presented in the first part. The second part contains three articles. The first paper has been submitted to Journal of Fluid Mechanics, the second paper to Physics of Fluids, and the third paper to Physical Review Letters.

The manuscripts are fitted to the present thesis format without changing any of the content.


November 2015, Stockholm

Walter Fornari
Division of work between authors
The main advisor for the project is Prof. Luca Brandt (LB). Prof. Minh Do-Quang (MD) acts as co-advisor.

Paper 1
The simulation code for interface resolved simulations developed by Wim-Paul Breugem (WB) was made tri-periodic by Walter Fornari (WF), who also introduced a forcing to create a sustained homogeneous isotropic turbulent field. Simulations and data analysis were performed by WF. The paper has been written by WF with feedback from LB and Prof. Francesco Picano (FP).

Paper 2
The computations were performed by Alberto Formenti (AF) with support from WF. Data analysis has been performed by WF and AF. The paper has been written by WF with feedback from LB and FP.

Paper 3
The computations have been performed by WF and Cyan Umbert López (CL). Data analysis has been performed in part by CL and mostly by WF. The paper has been written by Prof. Dhrubaditya Mitra (DB), WF and FP with feedback from LB and Pinaki Chaudhuri (PC).
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Part I

Overview and summary
CHAPTER 1

Introduction

Commonly in every day life, we tend to make the wrong assumption that all liquids behave in the same way, and that the main difference from one liquid to the other is just their viscosity (e.g. water, blood, honey). However these fluids often show different peculiar properties and behaviors that cannot be simply linked to their viscosities and this is because a solid phase is dissolved in them. Fluids in which particles are dispersed in a carrier gas or liquid are usually referred to as complex fluids since the linear relationship between the stress and the strain rate is lost.

Complex fluids are widely found in both nature and industrial applications. Environmental applications include sediment transport in surface water flows, water droplets, dust storms and pyroclastic flows. Other examples include suspended micro-organisms in water (such as plankton) and blood (where red blood cells confer a non-Newtonian behavior to the suspension). Typical engineering applications are instead oil, chemical and pharmaceutical processes and fluidized beds and soot particle dispersion.

From these examples it is easy to understand that different applications involve many different scenarios and flow regimes. First of all we can distinguish among bounded flows (channel, duct or pipe flows) and unbounded flows. We can then identify problems at different flow regimes. Some particles are small and fluid inertia at the particle scale is weak. In this situation the particle Reynolds number $Re_p$ tends to zero and the suspension is in the so-called Stockesian (or viscous) regime. As inertia increases, the suspension is first in the laminar regime and then, after the transition has occurred, in the fully turbulent regime. The Stockesian regime can be often found in microdevices while the turbulence scenario is often found in the atmosphere (either in ocean or in clouds during rain droplets formation). Furthermore, different type of particles can be identified based on their shape, size, density, deformability, and the suspension behavior strongly depends on the solid volume fraction (basically the fraction of the total volume occupied by the solid particles). In the so-called active fluids, these particles may even be capable of swimming, for example by sensing nutrient gradients (Lambert et al. 2013). The behavior of these complex fluids drastically changes depending on the abovementioned properties. For example when the suspensions are bounded it becomes very interesting to study their rheological properties (Stickel & Powell 2005; Morris 2009). Depending on the shear rate these suspensions may either exhibit shear thinning (a decrease in
the suspension effective viscosity), shear thickening (an increase of the effective viscosity) or other typical non-Newtonian behaviors (such as viscoelasticity). When the flow is turbulent, the presence of the solid phase may also lead to a modulation and modification of the turbulent field (Kulick et al. 1994; Zhao et al. 2010). Depending on the type and size of the particles, turbulent velocity fluctuations may be increased or decreased as well as the total flow drag. Due to the presence of walls also very interesting migrations may occur, which depend for example on the flow regime, on the type of particles and on the solid to fluid density ratio (Reeks 1983; Lashgari et al. 2015b). Interestingly, different cases may even lead to qualitatively similar migrations although the physical mechanisms behind them may be totally different.

When dealing with open environments, one of the most common problems investigated is sedimentation. In all of the previous examples, it is possible to easily define a fluid and a particle Reynolds number. When particles settle, their terminal falling velocity is usually unknown a priori and it becomes necessary to introduce a new non-dimensional number, the so-called Galileo or Archimedes number which quantifies the importance of the buoyancy forces acting on the particles with respect to viscous forces. Depending on the Galileo number, isolated particles exhibit different types of wakes and fall at different velocities (Uhlmann & Doychev 2014; Yin & Koch 2007). When suspensions are considered, clustering of particles may also occur depending on the particle-fluid interactions and the particle mean settling velocity may be different from the one expected for such a suspension (Uhlmann & Dušek 2014). Indeed in a quiescent fluid the mean settling velocity is typically a decreasing function of the solid volume fraction (Richardson & Zaki 1954). In dilute suspensions, one interesting fluid-particle interaction leads to the so-called Drafting-Kissing-Tumbling (DKT). If a spherical particle has a sufficiently long wake and an oncoming particle is entrained by it, the latter will be strongly accelerated (drafted) towards the former. The particles will then kiss and the particle behind will tumble towards one side (Fortes et al. 1987).

When sedimentation occurs in an already turbulent field, the interactions among eddies of different sizes and particles alter the whole process. Particles may fall on average faster or slower than in the quiescent fluid case (Wang & Maxey 1993; Good et al. 2014; Byron 2015). The increase or decrease in mean settling velocity can be up to 60%. Of course, the turbulent flow is also modulated and modified due to the energy injection at the particle scale.

The aim of this short summary is to give the reader a brief idea about the wide range of applications where complex fluids are involved and especially about the complexity of the problem. Many experimentally and numerically observed behaviors are still far from clear, and due to the wide range of parameters involved there is still much to explore in each of the different flow regimes. In the present work, three main different scenarios have been studied. Concerning unbounded flows, the settling of finite-size particles has been studied in both quiescent fluids and sustained homogeneous isotropic turbulence. Different volume fractions (between 0.5 and 1%) have been investigated and an effort was
made in order to understand the mechanisms leading to the different behaviors and settling velocities found in each case.

Up to date indeed, most of the works on sedimentation in turbulent environments have considered sub-Kolmogorov (Wang & Maxey 1993) or Kolmogorov size particles (where the Kolmogorov length and time scales are the scales of the smallest dissipative eddies) in the dilute regime (i.e. with very low volume fractions of the order of $10^{-5}$). When larger particles are considered (Lucci et al. 2010), the dynamics is strongly influenced by the ratios between the typical particle length and time scales (their diameter and the relaxation time) and those of the turbulent field (either the integral scales or the Kolmogorov, dissipative scales). Substantial amount of relative motion between particles and fluid is usually generated and predictions become almost prohibitive.

Regarding bounded flows, two cases at totally different flow regimes have been investigated. One study is devoted to the understanding of the behavior of a suspension of finite-size particles in a turbulent channel flow. The effect of varying the mass fraction and the solid-to-fluid density ratio has been studied in an idealized scenario where gravity is neglected. As in sedimentation, most of the previous studies concerned either very small and heavy particles or finite-size particles at low volume fractions (Reeks 1983; Sardina et al. 2011). A recent study showed that as the volume fraction of neutrally buoyant finite-size particles is increased from 0 to 20%, the overall drag is also increased due to the growth of the particle induced stresses (Picano et al. 2015). However, the case of neutrally buoyant particles is usually an idealized scenario (Prosperetti 2015). Therefore it is crucial to understand how the results change when suspensions with different density ratios and mass fractions are considered.

The last study is about the rheology of confined suspensions of rigid spheres in a simple Couette flow at low Reynolds numbers. Much effort has been devoted to understand the effect of varying the imposed shear rate and volume fraction, especially in the Stokesian regime (Einstein 1906; Morris 2009; Picano et al. 2013). However not much is known about the weakly inertial regime and the effects of confinement. The weakly inertial regime is becoming more and more relevant, especially due to its importance in microfluidic devices (Di Carlo 2009).

The purpose of this work is to study the behavior of suspensions of finite-size particles in yet unexplored (or partially explored) flow cases. In particular, we have focused on the effects of the ratio between the particle and fluid density and the confinement induced by the presence of walls.

In the following chapter, the governing equations describing the dynamics of the fluid and solid phases are discussed as well as the Immersed Boundary Method used for the direct numerical simulations (DNS). Next, the problems examined are more deeply discussed and finally, in the last chapter the main results are summarized and an outlook on future investigations is provided.
CHAPTER 2

Governing equations and numerical method

When dealing with complex fluids it is necessary to describe the coupled dynamics of both fluid and solid phases. Typically the fluid is treated as a continuum composed of an infinite number of fluid parcels. Each fluid parcel consists of an high number of atoms or molecules and is described by their averaged properties (such as velocity, temperature, density and so on).

Many applications deal with either liquids or gases with flow speed significantly smaller than the speed of sound (less than 30%). Under this condition, the fluid can be further assumed to be incompressible (i.e. the total volume of each fluid parcel is always constant). The final set of equations describing the motion of these fluids is known as the incompressible Navier-Stokes equations and reads

$$\nabla \cdot \mathbf{u}_f = 0 \quad (2.1)$$

$$\frac{\partial \mathbf{u}_f}{\partial t} + \mathbf{u}_f \cdot \nabla \mathbf{u}_f = -\frac{1}{\rho_f} \nabla p + \nu \nabla^2 \mathbf{u}_f \quad (2.2)$$

where $\mathbf{u}_f$, $\rho_f$, $\nu = \mu / \rho_f$ and $p$ are the fluid velocity, density, pressure and kinematic viscosity (while $\mu$ is the dynamic viscosity). Clearly, for the mathematical problem to be well-posed, suitable initial and boundary conditions must be assigned. When these equations are written in non-dimensional form, the inverse of the Reynolds number $Re = UL/\nu$ appears in front of the diffusive term on the right hand side of equation (2.2) (where $U$ and $L$ are a characteristic velocity and lengthscale of the system). The Reynolds number is a non-dimensional number that quantifies the importance of the inertial forces respect to the viscous forces in the specific problem. The Navier-Stokes equations are second order nonlinear partial differential equations and analytic solutions exist only for a very limited set of problems. Therefore, either experimental or numerical investigations are commonly carried out. As already stated, in the present work all the results have been obtained by direct numerical simulations.

When a solid phase is dispersed in the fluid, the Navier-Stokes equations must be coupled with the equations of motion for the solid particles. Assuming the particles to be non-deformable and spherical, the rigid body dynamics is described by a total of 6 degrees of freedom: translations in three directions and
rotations around three axis. The particles centroid linear and angular velocities, $\mathbf{u}_p$ and $\mathbf{\omega}_p$ are then governed by the Newton-Euler Lagrangian equations,

$$\rho_p V_p \frac{d\mathbf{u}_p}{dt} = \rho_f \int_{\partial V_p} \mathbf{\tau} \cdot \mathbf{n} \, dS + (\rho_p - \rho_f) V_p \mathbf{g}$$  \hspace{1cm} (2.3)$$

$$I_p \frac{d\mathbf{\omega}_p}{dt} = \rho_f \int_{\partial V_p} \mathbf{r} \times \mathbf{\tau} \cdot \mathbf{n} \, dS$$  \hspace{1cm} (2.4)$$

where $V_p = 4\pi a^3/3$ and $I_p = 2\rho_p V_p a^2/5$ are the particle volume and moment of inertia, with $a$ the particle radius; $\mathbf{g}$ is the gravitational acceleration; $\mathbf{\tau} = -p \mathbf{I} + 2\mu \mathbf{E}$ is the fluid stress, with $\mathbf{I}$ the identity matrix and $\mathbf{E} = \left( \nabla \mathbf{u}_f + \nabla \mathbf{u}_f^T \right) / 2$ the deformation tensor; $\mathbf{r}$ is the distance vector from the center of the sphere while $\mathbf{n}$ is the unit vector normal to the particle surface $\partial V_p$. To couple the motion of the distinct phases, it is then necessary to enforce Dirichlet boundary conditions for the fluid phase on the particle surfaces as $\mathbf{u}_f|_{\partial V_p} = \mathbf{u}_p + \mathbf{\omega}_p \times \mathbf{r}$.

Having described the mathematical problem, it is now time to describe the numerical method used to couple the dynamics of the fluid and solid phases. In particular, this is done by using the Immersed Boundary Method originally developed by Uhlmann (2005) and modified by Breugem (2012). In the numerical code, the boundary condition at the moving particle surface (i.e. $\mathbf{u}_f|_{\partial V_p} = \mathbf{u}_p + \mathbf{\omega}_p \times \mathbf{r}$) is modeled by adding a force field on the right-hand side of the Navier-Stokes equations. The fluid phase is therefore evolved in the whole computational domain using a second order finite difference scheme on a staggered mesh, without having to re-mesh at each time step to account for the particle position. The time integration is performed by a third order Runge-Kutta scheme combined with a pressure-correction method at each sub-step. The same integration scheme is also used for the Lagrangian evolution of eqs. (2.3) and (2.4). The forces exchanged by the fluid and the particles are imposed on $N_L$ Lagrangian points uniformly distributed on the particle surface. The force $\mathbf{F}_l$ acting on the $l-th$ Lagrangian point is related to the Eulerian force field $\mathbf{f}$ by the expression $\mathbf{f}(\mathbf{x}) = \sum_{l=1}^{N_L} \mathbf{F}_l \delta_d(\mathbf{x} - \mathbf{X}_l) \Delta V_l$ (where $\Delta V_l$ represents the volume of the cell containing the $l-th$ Lagrangian point while $\delta_d$ is the regularized Dirac delta). This force field is obtained through an iterative algorithm that maintains second order global accuracy in space. Using this IBM force field eqs. (2.3) and (2.4) are rearranged as follows to maintain accuracy,

$$\rho_p V_p \frac{d\mathbf{u}_p}{dt} = -\rho_f \sum_{l=1}^{N_L} \mathbf{F}_l \Delta V_l + \rho_f \frac{d}{dt} \int_{V_p} \mathbf{u}_f \, dV + (\rho_p - \rho_f) V_p \mathbf{g}$$  \hspace{1cm} (2.5)$$

$$I_p \frac{d\mathbf{\omega}_p}{dt} = -\rho_f \sum_{l=1}^{N_L} \mathbf{r}_l \times \mathbf{F}_l \Delta V_l + \rho_f \frac{d}{dt} \int_{V_p} \mathbf{r} \times \mathbf{u}_f \, dV$$  \hspace{1cm} (2.6)$$

where $\mathbf{r}_l$ is the distance from the center of a particle while the second terms on the right-hand sides are corrections to account for the inertia of the fictitious
fluid contained within the particle volume. This helps the numerical scheme to be stable even for neutrally buoyant particles.

Particle-particle and particle-walls interactions need to be considered. When the gap distance between two particles is smaller than twice the mesh size, lubrication models based on Brenner’s asymptotic solution (Brenner 1961) are used to correctly reproduce the interaction between the particles. A soft-collision model is used to account for particle-particle and particle-wall collisions with an almost elastic rebound (the restitution coefficient is 0.97). These lubrication and collision forces are added to the right-hand side of eq. (2.5). More details and validations of the numerical code can be found in Breugem (2012) and Lambert et al. (2013).

In the following chapters, the problems studied in the context of this work are more thoroughly discussed. Up to date theoretical, numerical and experimental findings on the topics are reviewed, highlighting everytime the yet unknown facts and aspects.
CHAPTER 3

Settling of finite-size particles

The problem of sedimentation has been widely studied during the years due to its importance in a wide range of natural and engineering applications. One of the earliest investigations on the topic was Stokes’ analysis of the sedimentation of a single rigid sphere through an unbounded quiescent viscous fluid at zero Reynolds number. Under this conditions, the motion of the particle is always steady (there are no accelerations) and the sedimentation velocity \( V_s \) can easily be found by balancing the drag \( (F^D = 6\pi \mu a V_s) \) and the buoyancy forces acting on the particle (Guazzelli & Morris 2012). The sedimentation velocity can therefore be expressed as

\[
V_s = \frac{2 a^2}{9 \mu} (\rho_p - \rho_f) g = \frac{2 a^2}{9 \nu} (R - 1) g \quad (3.1)
\]

where \( R = \rho_p / \rho_f \) is the solid-to-fluid density ratio. In a viscous flow the sedimentation velocity \( V_s \) of an isolated particle is directly proportional to the square of its radius \( a \), to the density ratio \( R \) and to the gravitational acceleration \( g \), while it is indirectly proportional to the fluid viscosity \( \nu \). However this result is limited to the case of a single particle in Stokes flow and corrections must be considered to account for the collective effects and inertia \( (Re > 0) \).

Under the assumption of very dilute suspensions and Stokes flow, Hasimoto (1959) and later Sangani & Acrivos (1982) obtained expressions for the drag force exerted by the fluid on three different cubic arrays of rigid spheres. These expressions relate the drag force only to the solid volume fraction \( \phi \). For example, in the case of a simple cubic lattice the mean settling velocity \( v_t \) of a very dilute suspension can be expressed as

\[
|v_t| = |V_s| \left[ 1 - 1.7601 \phi^{1/3} + O(\phi) \right] \quad (3.2)
\]

A different approach was pursued by Batchelor & Green (1972), who found another expression for the mean settling velocity using conditional probability arguments:

\[
v_t = V_s |1 - 6.55\phi| \quad (3.3)
\]

When the Reynolds number of the settling particles \( (Re_t = 2a|v_t|/\nu) \) becomes finite, the assumption of Stokes flow is less acceptable (especially for \( Re_t > 1 \)) and solutions should be derived using the Navier-Stokes equations. However due to the nonlinearity of the inertial term, the analytical treatment of
such problems is extremely difficult and theoretical investigations have progressively given way to experimental and numerical approaches. Current theoretical works focus mostly on the spatial patterns of inertial particles in turbulence (Gustavsson & Mehlig 2014).

The first remarkable experimental results obtained for creeping flow and small Reynolds numbers were those by Richardson & Zaki (1954). They proposed an empirical formula relating the mean settling velocity of a suspension to its volume fraction $\phi$ and to the settling velocity of an isolated particle

$$ |v_t| = |V_s| [1 - \phi]^n $$

(3.4)

where $n$ is a coefficient usually taken to be 5.1 (while $V_s$ is the measured velocity of a single particle and therefore not necessarily its Stokes approximation). The Richardson-Zaki formula is believed to be accurate also for concentrated suspensions (up to a volume fraction $\phi$ of about 25%) and has been subsequently improved to cover also the intermediate Reynolds number regime (Garside & Al-Dibouni 1977; Di Felice 1999). More recently, Yin & Koch (2007) performed direct numerical simulations of settling finite-size particles using a Lattice-Boltzmann method in the low and intermediate Reynolds number regime (up to $Re_t = 20$), and suggested to add a premultiplying factor $\alpha$ to the right hand side of the Richardson-Zaki formula, where $\alpha$ varies between 0.86 and 0.92.

In the inertial regime, however, the settling velocity is generally unknown a priori and it is difficult to properly define the particle Reynolds number. Thus, the non-dimensional number often used to characterize the settling process is the Archimedes or Galileo number

$$ Ga = \sqrt{(R - 1)g(2a)^3} \mu $$

(3.5)

namely the ratio between buoyancy and viscous forces. Particles with different Galileo numbers $Ga$ fall at different speeds and exhibit different wake regimes (Bouchet et al. 2006; Uhlmann & Dušek 2014). Indeed as $Ga$ is increased, the wake undergoes various bifurcations shifting from the steady axi-symmetric regime to the chaotic regime (through various intermediate regimes). The Galileo number $Ga$ also directly affects the behavior of a suspension of settling particles. For example Uhlmann & Doychev (2014) showed that above a specific $Ga$, clustering of finite-size particles occurs and surprisingly, a suspension with $\phi = 0.5\%$ settles on average faster than a single isolated particle. Indeed due to the hindrance effect (substantial amount of fluid moving in the opposite direction of falling particles due to the presence of a bottom wall), the mean settling velocity is generally reduced respect to the terminal velocity of a single particle. The reduction is higher for denser suspensions, as can be seen for example through the Richardson-Zaki formula.

The problem becomes even more complex when the particles are suspended in a turbulent field. Indeed in a turbulent flow, many different spatial and temporal scales are active and the motion of a particle does not depend only on its dimensions and characteristic response time, but also on the ratios among
these and the characteristic turbulent length and time scales. The turbulent quantities usually considered are the Kolmogorov length and time scales ($\eta = (\nu^3/\epsilon)^{1/4}$ and $t_\eta = (\nu/\epsilon)^{1/2}$ where $\epsilon$ is the energy dissipation) which are related to the smallest eddies. Alternatively, the integral lengthscale ($L_0 = k^{3/2}/\epsilon$ where $k$ is the turbulent kinetic energy) and the eddy turnover time ($T_e = k/\epsilon$) can also be used.

For the case of a small rigid sphere settling in a nonuniform flow, an equation of motion was derived already in the late 40′s and 50′s by Tchen (1947) and later Corrsin & Lumley (1956). In the derivation, they assumed the particle Reynolds number to be very low so that the viscous Stokes drag for a sphere could be applied. The added mass (the volume of surrounding fluid accelerated by the moving particle) and the augmented viscous drag due to a Basset history term were also included. Later Maxey & Riley (1983) corrected these equations including also the appropriate Faxen forces due to the unsteady Stokes flow. The final form of this equation is often referred to as the Maxey-Riley equation and reads:

$$\frac{4}{3} \pi a^3 \rho_p \frac{dV_p}{dt} = \frac{4}{3} \pi a^3 (\rho_p - \rho_f) g + \frac{4}{3} \pi a^3 \rho_f \frac{Du_f}{Dt} \bigg|_{x_c}$$

$$- 6\pi a \mu [V_p - u_f(x_c,t)] - \chi \frac{4}{3} \pi a^3 \rho_f \frac{d}{dt} [V_p - u_f(x_c,t)]$$

$$- 6\pi a^2 \mu \int_0^t \left( \frac{d}{d\tau} [V_p - u_f(x_c,t)] \right) d\tau \quad (3.6)$$

where $\chi = 0.5$ is the added mass coefficient, $D/Dt|_{x_c} = (\partial/\partial t + u_f \cdot \nabla)$ is a time derivative following a fluid element, while $d/dt = (\partial/\partial t + V_p \cdot \nabla)$ is a time derivative following the moving sphere. The terms on the right hand side of equation 3.6 are the buoyancy force, the stress-gradient force (related to the pressure gradient of the undisturbed flow), the viscous Stokes drag, the force due to the added mass and the Basset history force. For simplicity the Faxen corrections have been neglected in the last three terms.

The Maxey-Riley equation can then be extended to the case of low particle Reynolds numbers by using empirical nonlinear drag corrections (Schiller & Naumann 1935) such as

$$C_D = \frac{24}{Re_p} \left( 1 + 0.1935 Re_p^{0.6305} \right) \quad (3.7)$$

(where $C_D = 24/Re_p$ is the drag coefficient for a sphere in Stokes flow), and by changing the integration kernel of the history force, e.g. as proposed by (Mei & Adrian 1992). Recently Loth & Dorgan (2009) tried to extend equation 3.6 to account for finite particle size by means of spatial-averaging of the continuous flow properties.

The main problem of the Maxey-Riley equation is that it is related to the motion of a single particle and it cannot be used to study the settling of dense suspensions in turbulent flows.

The cases usually studied numerically with the Maxey-Riley equation are the
sedimentation of very dilute suspensions of small (either sub-Kolmogorov or Kolmogorov size) heavy particles, with low mass loadings. This is usually known as the one-way coupling regime (Balachandar & Eaton 2010) since there is no back-reaction on the fluid phase and the flow field is unaltered. Instead, when the mass loading becomes important the back-reaction due to the solid phase must be considered and we enter the so-called two-way coupling regime.

For dilute suspensions of small heavy particles it has been shown that turbulence can either enhance, reduce or inhibit the settling. Weakly inertial particles may be indefinitely trapped in a forced vortex (Tooby et al. 1977) but as particle density increases, their settling speeds may be increased due to the transient nature of turbulence. Highly inertial particles tend indeed to move outward from the center of eddies and are often swept into regions of downdrafts (the so called preferential sweeping or fast-tracking). In doing so, the particle mean settling velocity is increased with respect to the quiescent case. This was first observed numerically by Wang & Maxey (1993) who studied the settling of a dilute suspension of heavy point-particles (i.e. one-way coupled) in homogeneous isotropic turbulence, and confirmed by various experiments (Nielsen 1993; Aliseda et al. 2002; Yang & Shy 2003, 2005). In the two-way coupling regime, the mean settling velocity is further increased as shown by Bosse et al. (2006).

However the particle mean settling velocity can also be reduced respect to that in quiescent fluid. Such behavior has been observed in both experiments (Murray 1970; Nielsen 1993; Yang & Shy 2003; Kawanisi & Shiozaki 2008) and simulations Wang & Maxey (1993); Good et al. (2014), and it is only possible when the particle Reynolds number is greater than zero. This implies that in numerical simulations, the mean settling velocity reduction is obtained only if nonlinear drag corrections are included (Good et al. 2014). Nielsen (1993) suggested that fast-falling particles that bisect both downward- and upward-moving flow regions, need a longer time to cross the latter (a phenomenology usually referred to as loitering), especially if the particles settling speed is similar to the turbulence velocity fluctuations $u'$. When finite-size particles are considered, we are typically in the four-way coupling regime since both mass loading and volume fraction are high and also interactions among particles must be considered. Due to the difficulty of dealing with these interactions, there are up to date very few studies on the settling of such particles in turbulent flows.

Among experimental studies it is certainly worth mentioning the one by Byron (2015) who investigated the settling of Taylor-scale particles in turbulent aquatic environments using a Refractive-Index-Matched Hydrogel Method PIV (Particle Image Velocimetry). The authors found that particles with quiescent settling velocities of the same order of the turbulent rms velocity $u'$, fall on average 40 – 60% more slowly than in quiescent fluid (depending on their density and shape). However the reason behind the mean velocity reduction remains unclear. The overall drag acting on the particles could be
increased either by stronger nonlinear effects due to the substantial amount of relative motion generated among phases (Stout et al. 1995), or by important unsteady history effects (Mordant & Pinton 2000; Sobral et al. 2007; Olivieri et al. 2014; Bergougnoux et al. 2014).

Other interesting aspects that should be explored are for example one- and two-particle dispersions, particle velocity correlations, particle wakes, collision rates and turbulence modulation at different Galileo numbers $Ga$ and solid volume fractions $\phi$.  ```
CHAPTER 4

Particles in shear flows

4.1. Stokesian and laminar regimes

Understanding the rheological properties of suspensions in shear flows is not only a challenge from a theoretical point of view but has also an impact in many industrial applications. Even restricting the analysis to monodisperse rigid neutrally buoyant spheres in the viscous or laminar regime, the flow of these suspensions shows peculiar rheological properties such as shear thinning or thickening, normal stress differences and jamming at high volume fractions (Stickel & Powell 2005; Morris 2009). Indeed the suspended phase alters the response of the complex fluid to the local deformation rate leading, for example, to an increase of the effective viscosity of the suspension $\mu_e$ with respect to that of the pure fluid.

The earliest works in the field were those by Einstein (1906, 1911) who derived an expression to calculate the effective viscosity of a suspension under the assumptions of Stokes flow and very low volume fractions. This expression, usually termed as Einstein viscosity, reads

$$\mu_e = \mu \left(1 + \frac{5}{2} \phi \right)$$

and shows that the normalized viscosity $\mu_e/\mu$ grows linearly with the volume fraction $\phi$. Due to the assumptions adopted in the derivation, equation 4.1 is valid only for $\phi < 0.05$. For higher volume fractions, equation 4.1 underpredicts the effective viscosity $\mu_e$ since it does not account for particle interactions that would yield a viscosity contribution of $O(\phi^2)$. The $O(\phi^2)$ correction has been found for pure straining flow by Batchelor & Green (1972).

The mutual interactions between particles become increasingly critical when increasing the volume fraction. In the denser regime the effective viscosity increases by more than one order of magnitude until the system jams behaving as a glass or crystal (Sierou & Brady 2002). As the system approaches the maximum packing limit ($\phi_m = 0.58 - 0.62$) the effective viscosity of the suspension diverges (Boyer et al. 2011). This behavior is properly reproduced by empirical fits such as those by Eilers and Kriegher & Dougherty (Stickel & Powell 2005).

The suspension effective viscosity is also altered by changing the imposed shear rate $\dot{\gamma}$. As the shear rate increases, the suspension shear thins from a zero-shear rate plateau viscosity until a minimum is reached. Further
increasing the shear rate leads to shear thickening of the suspension (Stickel & Powell 2005). The viscosity of suspensions may also exhibit time-dependent behavior. For example, when a steady shear is imposed on thixotropic materials, the viscosity decreases with time until it reaches an asymptotic value. However after a period at rest, the suspension will recover its initial viscosity. When the shear rate is changed, these materials also show a time-dependent stress response. Thixotropy is believed to be related to a shear-induced change in the microstructure of the material (Guazzelli & Morris 2012).

Changes in volume fraction and shear rate may also induce normal stress differences in dense suspensions of hard spheres, especially when $\phi > 0$. In a Newtonian fluid, linear shear flow generates no normal stresses $\sigma_{ii}$ since there is no pressure response. However a suspension in shear flow exerts normal stresses that can be different in each direction. Therefore the normal stress in a shear suspension loses isotropy and normal stress differences can be defined as $N_1 = \sigma_{xx} - \sigma_{yy}$ and $N_2 = \sigma_{yy} - \sigma_{zz}$ (in a frame of reference where $u_x = \dot{\gamma} y$).

Similar rheological behaviors can also be observed in the weakly inertial regime (Kulkarni & Morris 2008b; Picano et al. 2013; Zarraga et al. 2000). Indeed when the particle Reynolds number ($Re_p = \dot{\gamma} a^2 / \nu$) is finite, the symmetry of the particle pair trajectories is broken and the microstructure becomes anisotropic inducing shear thickening and normal stress differences. Recently Picano et al. (2013) showed that at finite inertia the microstructure anisotropy results in the formation of shadow regions with no relative flux of particles. Due to these shadow regions, the effective volume fraction increases and shear thickening occurs. However the understanding of such flows is still far from complete and research on the field is very active. In this work we study the effect of confinement on the rheology of a dense suspension of neutrally buoyant hard spheres ($\phi = 0.3$) in the low inertial regime.

4.2. Turbulent regime

Concerning the highly inertial regime, the seminal work of Bagnold (1954) revealed that the effective viscosity $\mu_e$ increases linearly with the shear rate $\dot{\gamma}$ due to the increase of collisions among particles. Further increasing the Reynolds number, inertial effects become more important until the flow undergoes a transition to the turbulent regime. This is generally the case for unladen flows while the transition may be inhibited for suspensions at very high volume fractions $\phi$.

In wall-bounded turbulent flows it is generally possible to identify an outer lengthscale (typically the boundary layer thickness or the channel half-width $h$) and an inner lengthscale typical of a region in which viscous effects are significant (Pope 2000). The inner lengthscale is expressed as $\delta_* = \nu / U_*$ where $U_* = \sqrt{\tau_w / \rho_f}$ is the friction velocity, while $\tau_w$ is the wall-shear stress (due to the no-slip boundary condition at the wall). Using these we can define the
friction Reynolds number as $$Re_\tau = U_* h / \nu$$.

Inside the inner region it is then possible to identify a viscous sublayer (very close to the wall), a buffer layer and a log-layer. In this last layer, the mean streamwise velocity profile grows as the natural logarithm of the wall-distance scaled in inner units ($y^+ = y / \delta_*$)

$$U^+_x = \frac{U_x}{U_*} = \frac{1}{\kappa} \ln y^+ + B$$  \hspace{1cm} (4.2)

where $$U_x$$ is the mean streamwise velocity, $$\kappa$$ is the von Kármán constant and $$B$$ is an additive coefficient. This self-similar solution is known as the "law of the wall". Drag is directly linked to this mean velocity profile. Typically a decrease in $$\kappa$$ denotes drag reduction while small or negative $$B$$ lead to an increase in drag (Virk 1975).

When small and heavy particles are suspended in the turbulent flow (one-way coupling regime), they tend to migrate from regions of high to low turbulence intensities, i.e. toward the wall (Reeks 1983). This phenomenon is known as turbophoresis and it is stronger when the turbulent near-wall characteristic time and the particle inertial time scale are similar (Soldati & Marchioli 2009). However more recent numerical results showed that also small-scale clustering occurs and together with turbophoresis this leads to the formation of streaky particle patterns (Sardina et al. 2011, 2012).

When the mass loading of the particles becomes sufficiently high, we access the two-way coupling regime (i.e. the back-reaction of the dispersed phase on the fluid must be considered). In a turbulent channel flow, the spherical particles reduce the turbulent near wall fluctuations in the spanwise and wall-normal directions, while the streamwise velocity fluctuation and mean velocity are enhanced. Therefore drag reduction is achieved in a fashion similar to that obtained by using polymeric or fiber additives (Zhao et al. 2010). However when particles larger than the dissipative lengthscale are considered, both turbulence intensities and Reynolds stress ($$\langle u_x u_y \rangle$$) are increased (Pan & Banerjee 1996).

When the volume fraction $$\phi$$ of these finite-size particles is sufficiently high, all the possible interactions among particles must be considered.

Concerning turbulent channel flows, Shao et al. (2012) showed that a semi-dilute suspension of neutrally buoyant spheres ($$\phi \simeq 7\%$$) attenuates the large-scale streamwise vortices and reduces fluid streamwise velocity fluctuations (except in regions very close to the walls or around the centerline). On the other hand, the particles increase the spanwise and wall-normal velocity fluctuations in the near-wall region by inducing small scale vortices.

More recently, Picano et al. (2015) observed that as the volume fraction $$\phi$$ of a suspension of rigid neutrally buoyant particles is increased from 0% to 20%, also the overall drag is increased. Interestingly, the drag is higher at the highest volume fraction ($$\phi = 20\%$$) although the turbulence intensities and the Reynolds shear stresses are importantly reduced. However, analyzing the mean momentum balance it is possible to obtain the following equation for the total stress $$\tau(y)$$ in a turbulent channel flow laden with finite-size neutrally buoyant
4.2. TURBULENT REGIME

particles

\[
\tau(y) = \rho_f \left( u_{c,x} u_{c,y}' \right) + \nu (1 - \phi) \frac{dU_{f,x}}{dy} + \frac{\phi}{\rho_f} \langle \sigma_{p,xy} \rangle = \nu \left. \frac{dU_{f,x}}{dy} \right|_w \left( 1 - \frac{y}{h} \right) \quad (4.3)
\]

(where \( \nu \left. \frac{dU_{f,x}}{dy} \right|_w \) is the stress at the wall \( \tau_w \)). Equation 4.3 shows that the total stress is given by three contributions: the viscous part \( \tau_V / \rho_f = \nu (1 - \phi) \frac{dU_{f,x}}{dy} \), the turbulent part \( \tau_T / \rho_f = -\langle u_{c,x} u_{c,y}' \rangle = -(1 - \phi) \langle u_{f,x} u_{f,y}' \rangle - \phi \langle u_{p,x} u_{p,y}' \rangle \) and the particle induced stress \( \tau_P / \rho_f = \phi \langle \sigma_{p,xy} / \rho_f \rangle \). Picano et al. (2015) found that at the highest volume fraction, although the Reynolds stress is reduced, the particle induced stress is drastically increased leading also to an increase in overall drag. The increase in drag is therefore not associated to a turbulence enhancement but to an increase of the effective viscosity of the suspension.

Based on different volume fractions \( \phi \) and Reynolds numbers, Lashgari et al. (2014) further identified three different regimes (laminar, turbulent and shear thickening regimes) in which the flow is dominated by one of the different components of the total stress.

In the present work, we consider a turbulent channel flow laden with finite-size rigid particles and we change the volume fraction \( \phi \) and density ratio \( R \) in an idealized scenario where gravity is neglected. The main scope is to understand independently the effects of excluded volume (i.e. of \( \phi \)) and particle inertia (\( R \)) on the statistical observables of both fluid and solid phases.

In the next chapter the main findings of the works on sedimentation, channel flow and confined rheology are summarized.
CHAPTER 5

Summary of the papers

Paper 1

*Sedimentation of finite-size spheres in quiescent and turbulent environments.*

Particle sedimentation is encountered in a wide number of applications and environmental flows. It is a process that usually involves a high number of particles settling in different environments. The suspending fluid can either be quiescent or turbulent while particles may differ in size, shape, density and deformability. Owing to the range of spatial and temporal scales generally involved, the interaction between the fluid and solid phases is highly complex and the global properties of these suspensions can be substantially altered from one case to another. Although sedimentation has always been an active field of research, yet little is known about the settling of finite-size particles in homogeneous isotropic turbulence.

In this work we performed Direct Numerical Simulations of sedimentation in quiescent and turbulent environments using an Immersed Boundary Method to account for the solid phase. We considered a suspension of rigid spheres with diameter of about 12 Kolmogorov length scales $\eta$ and solid to fluid density ratio $R = 1.02$. Based on these values, the Galileo number $Ga$ of the particles was about 145. Two solid volume fractions were investigated ($\phi = 0.5\%$ and $1\%$). An unbounded computational domain with tri-periodic boundary conditions was used ensuring at each time step a zero total mass flux. For the turbulent cases, an homogeneous isotropic turbulent field was generated and sustained using a $\delta$-correlated in time forcing of fixed amplitude. The achieved Reynolds number based on the Taylor microscale $Re\lambda = \lambda u' / \nu$ (where $\lambda$ is the Taylor microscale and $u'$ is the turbulence rms velocity) was about 90. Comparing the results obtained in quiescent fluid and homogeneous isotropic turbulence we found the striking result that finite-size particles tend to settle more slowly in the turbulent environments. The mean settling velocity is reduced by about 8.5\% respect to the quiescent cases for both volume fractions. The reduction respect to the isolated particle in quiescent fluid is about 12 and 14\% for $\phi = 0.5\%$ and $1\%$. We also examined the probability density functions ($pdf$s) of the particle velocities in the directions parallel and perpendicular to gravity. In the direction of gravity, the $pdf$s are found to be almost Gaussian in
the turbulent cases while large positive tails are found in the quiescent cases. In the latter, the pdf’s are positively skewed and the flatness is much higher than 3. The tails are due to the intermittent fast sedimentation of particle pairs in drafting-kissing-tumbling motions (DKT). The DKT is highly reduced in the turbulent cases since the particle wakes are quickly disrupted by the turbulent eddies.

Particle velocity autocorrelations and single particle dispersions were also examined. It is found that particle velocity fluctuations decorrelate faster in homogeneous isotropic turbulence. Particle lateral dispersion is found to be higher in the turbulent cases while the vertical one is found to be of comparable magnitude for all cases examined. However in the quiescent case at lowest volume fraction ($\phi = 0.5\%$), longer times are needed before the diffusive behavior is reached.

Finally, by analyzing the particle relative velocities it is found that the reduction in mean settling velocity found in the turbulent cases is due to unsteady effects (such as vortex shedding) which increase the total drag acting on the particles.

**Paper 2**

*The effect of particle density in turbulent channel flow laden with finite size particles in semi-dilute conditions.*

Suspensions of finite-size particles are also found in many applications which involve wall-bounded turbulent flows. Concerning turbulent channel flows, it has been shown that the presence of a dispersed phase may alter the near-wall turbulence intensities and Reynolds stress. Therefore streamwise coherent structures are modified and drag is either enhanced or reduced.

It has been shown that increasing the volume fraction $\phi$ of a suspension of neutrally buoyant spheres in a turbulent channel flow leads to an increase of the total drag. This is due to the increase of the particle induced stress at higher volume fractions, while the turbulent stresses are reduced. However, little is known about the importance of particle inertia and therefore of the solid to fluid density ratio $R$. Here we performed Direct Numerical Simulations of a turbulent channel flow laden with finite-size rigid spheres. The imposed bulk Reynolds number $Re_b = 2hU_0/\nu$ of the reference unladen case was chosen to be 5600 (with $U_0$ being the bulk velocity), giving a friction Reynolds number $Re_\lambda$ of about 180. The ratio between the particle radius and the channel half-width was fixed to $a/h = 1/18$. Two sets of simulations were initially performed. First the mass fraction $\chi$ was kept constant while changing both volume fraction $\phi$ and density ratio $R$. Then, the volume fraction $\phi$ was kept fixed at 5% while the density ratio was increased from $R = 1$ to 10. In this idealized study, we neglected gravity and investigated the importance of excluded volume ($\phi$) and particle inertia ($R$) on the behavior of the suspension.
We found that both fluid and solid phase statistics are substantially altered by changes in volume fraction $\phi$, while up to $R = 10$ the effect of the density ratio is minimal. Increasing the volume fraction drastically changes the mean fluid velocity profiles and the fluid velocity fluctuations. Respect to the unladen case, the mean streamwise velocity is found to decrease close to the walls and increase around the centerline. Fluid velocity fluctuations are found to increase very close to the walls and to substantially decrease in the log-layer. In the cases at constant $\phi$, the results at higher $R$ are found to be very similar to those of the neutrally buoyant case.

The main result found at constant $\phi$ is a shear-induced migration toward the centerline. This behavior is shown to be more important at the highest density ratio ($R = 10$) and it is therefore a purely inertial effect.

Finally, we kept the volume fraction fixed at $\phi = 5\%$ and increased the density ratio to $R = 100$. We found that under these conditions, the solid and fluid phases decouple. In particular, the solid phase behaves as a dense gas and moves with an uniform streamwise velocity across the channel. Both particle and fluid velocity fluctuations are drastically reduced. Furthermore, the pdf of the modulus of the particle velocity fluctuations closely resembles a Maxwell-Boltzmann distribution typical of gaseous systems. In this regime, we also found that the collision rate is high and governed by the normal relative velocity among particles.

**Paper 3**

*Rheology of extremely confined non-Brownian suspensions.*

Suspensions of solid particles in simple shear flows show different rheological behaviors depending on their size, shape, volume fraction $\phi$, solid to fluid density ratio $R$ and imposed shear rate $\dot{\gamma}$. Typical rheological properties include normal stress differences, shear thinning or thickening, thixotropy and jamming at high volume fractions.

It has been shown that in the weakly intercel regime, the symmetry of the particle pair trajectories is broken inducing an anisotropic microstructure that in turn leads to shear thickening in a dense suspension of rigid spheres. Recently, intriguing confinement effects have been discovered for suspensions of spheres in the Stokesian regime. However nothing is known up to date about the effect of confinement at low but finite particle Reynolds numbers.

In this work we studied the rheology of extremely confined suspensions of rigid spherical (non-Brownian) particles by performing Direct Numerical Simulations. We considered a plane-Couette flow seeded with neutrally buoyant spheres. The suspension volume fraction is fixed at $\phi = 30\%$ and the confinement is studied by changing the dimensionless ratio $\xi = L_z/(2a)$, where $L_z$ is the channel width. In particular, the channel width is decreased from 6 to 1.5 particle diameters. The simulations are performed at three different particle Reynolds numbers $Re = \rho_f \dot{\gamma}a^2/\mu = 1, 5$ and 10.
The most striking result that we have found, is that the effective viscosity of the suspension does not show a monotonic behavior with decreasing $\xi$, but rather a series of maxima and minima. Interestingly the minima are found when the channel width is approximately an integer number of particle diameters. At these $\xi$ indeed, particle layering occurs and wall-normal migrations are drastically reduced. When layering occurs, the pdf of the particle wall-normal displacement is shown to possess exponential tails indicating a non-diffusive behavior. The typical diffusive behavior is instead recovered at intermediate $\xi$ (i.e. when there is no layering). This is also reflected in the particle mean squared wall-normal displacement. When there is no layering, the mean squared displacement grows linearly in time; however for integer values of $\xi$, it follows a power-law of the form $\sim t^{\beta}$ with $\beta < 1$.

Finally it is found that the motion of the particles relative to these layers is dynamically frozen.
In the present work we have investigated suspensions of rigid spherical particles in different applications.

We started by studying the settling of a semi-dilute suspension of finite-size spheres in both quiescent and turbulent environments. We showed that the mean settling velocity is reduced in the latter due to a reduction in drafting-kissing-tumbling events and to the appearance of important unsteady effects that increase the total drag.

Then we focused on wall-bounded flows. First we investigated a turbulent channel flow laden with finite-size particles. We studied the effects of varying the solid volume fraction and the solid to fluid density ratio in an idealized scenario where gravity is neglected. We found that fluid and particle statistics are mostly altered by changes in volume fraction while increasing the density ratio results in a shear-induced migration of particles toward the center of the channel. However, at very high density ratios ($R = 100$) fluid and solid phases decouple and the latter starts behaving as a dense gas.

Finally, we studied the rheology of extremely confined suspensions in simple shear flow. We considered a plane-Couette flow seeded with neutrally buoyant spheres in the weakly inertial regime. We found that as confinement is increased, the effective viscosity of the suspension shows minima when the channel width is approximately an integer number or particle diameters. At these channel widths, layering of particles occurs and wall-normal migrations are drastically reduced.

In the first paper about sedimentation we considered volume fractions of 0.5 and 1%, and we started investigating the turbulence modulation due to the solid phase. Next step will be to study suspensions at higher volume fractions and to examine more deeply the modification of the turbulent field. We will look more in detail at structure functions, fluid-particle energy exchange, spectra of energy dissipation, turbulence kinetic energy, energy transfer and frequency, as well as other typical quantities of homogeneous isotropic turbulent flows. The results will then be compared to those of the unladen case. In addition, it may also be interesting to examine the effect of different stochastic forcings.

It will also be interesting to investigate suspensions of finite-size non-spherical particles such as prolate and oblate ellipsoids. Due to the anisotropic geometry results will most probably drastically change for both sedimentation and
turbulent channel flows. Recently we have also modified the numerical code to account for polydisperse suspensions, that will be studied in similar flow cases.
Acknowledgements

I would like to thank Prof. Luca Brandt for accepting me as a Ph.D. student and for constantly helping me with plenty of suggestions, ideas and discussions on the different topics. I would also like to thank Prof. Dhrubaditya Mitra and Prof. Francesco Picano for spending time working with me, explaining and teaching me much, and the other collaborators: Pinaki Chaudhuri and the two former Master students, Cyan Umbert López and Alberto Formenti.

Then I would like to thank past and present colleagues in the department for joyful and interesting discussions or for bringing happiness by simply saying "Hello, hello".

Special thanks to all of my friends who never left me alone even when I wanted to be on my own. Among them I am obliged to mention two from Italy, Luigi Della Corte and Daniel Ferretti (since I owe it to them), some from "Sweden": Domenico, Matteo, Ricardo, Jacopo, Mehdi, Andrea, Freddy, Iman, JC, Emanuele, Prabal (among others); and those who came back to their countries: Matt, Yuki and Werner.

Finally my biggest gratitude goes to my family who always supported me, never expecting anything particular from me if not my serenity and happiness.


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Part II

Papers
Paper 1
Sedimentation of finite-size spheres in quiescent and turbulent environments

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Accepted in J. Fluid Mech.

Sedimentation of a dispersed solid phase is widely encountered in applications and environmental flows, yet little is known about the behavior of finite-size particles in homogeneous isotropic turbulence. To fill this gap, we perform Direct Numerical Simulations of sedimentation in quiescent and turbulent environments using an Immersed Boundary Method to account for the dispersed rigid spherical particles. The solid volume fractions considered are $\phi = 0.5 - 1\%$, while the solid to fluid density ratio $\rho_p/\rho_f = 1.02$. The particle radius is chosen to be approximately 6 Kolmogorov lengthscales. The results show that the mean settling velocity is lower in an already turbulent flow than in a quiescent fluid. The reduction with respect to a single particle in quiescent fluid is about 12% and 14% for the two volume fractions investigated. The probability density function of the particle velocity is almost Gaussian in a turbulent flow, whereas it displays large positive tails in quiescent fluid. These tails are associated to the intermittent fast sedimentation of particle pairs in drafting-kissing-tumbling motions. The particle lateral dispersion is higher in a turbulent flow, whereas the vertical one is, surprisingly, of comparable magnitude as a consequence of the highly intermittent behavior observed in the quiescent fluid. Using the concept of mean relative velocity we estimate the mean drag coefficient from empirical formulas and show that non stationary effects, related to vortex shedding, explain the increased reduction in mean settling velocity in a turbulent environment.

1. Introduction

The gravity-driven motion of solid particles in a viscous fluid is a relevant process in a wide number of scientific and engineering applications (Guazzelli & Morris 2012). Among these we recall fluvial geomorphology, chemical engineering systems, as well as pollutant transport in underground water and settling of micro-organisms such as plankton.

The general problem of sedimentation is very complex due to the high number
of factors from which it depends. Sedimentation involves large numbers of particles settling in different environments. The fluid in which the particles are suspended may be quiescent or turbulent. Particles may differ in size, shape, density and stiffness. The range of spatial and temporal scales involved is wide and the global properties of these suspensions can be substantially different from one case to another. Because of these complexities, our general understanding of the problem is still incomplete.

1.1. Settling in a quiescent fluid

One of the earliest investigations on the subject at hand is Stokes’ analysis of the sedimentation of a single rigid sphere through an unbounded quiescent viscous fluid at zero Reynolds number. This led to the well-known formula that links the settling velocity to the sphere radius, the solid to fluid density ratio and the viscosity of the fluid that bears his name. Later, the problem was studied both theoretically and experimentally. Hasimoto (1959) obtained expressions for the drag force exerted by the fluid on three different cubic arrays of rigid spheres. These relate the drag force only to the solid volume fraction, but were derived under the assumption of very dilute suspensions and Stokes flow. The formulae have later been revisited by Sangani & Acrivos (1982). A different approach was instead pursued by Batchelor & Green (1972) who found a relation between the mean settling velocity and the solid volume fraction by using conditional probability arguments. When the Reynolds number of the settling particles ($Re_t$) becomes finite, the assumption of Stokes flow is less acceptable (especially for $Re_t > 1$). The fore-aft symmetry of the fluid flow around the particles is broken and wakes form behind them. Solutions should be derived using the Navier-Stokes equations, but the nonlinearity of the inertial term makes the analytical treatment of such problems extremely difficult. For this reason theoretical investigations have progressively given way to experimental and numerical approaches.

The first remarkable experimental results obtained for creeping flow were those by Richardson & Zaki (1954). These authors proposed an empirical formula relating the mean settling velocity of a suspension to its volume fraction and to the settling velocity of an isolated particle. This formula is believed to be accurate also for concentrated suspensions (up to a volume fraction $\phi$ of about 25%) and for low Reynolds numbers. Subsequent investigations improved the formula so that it could also be applied in the intermediate Reynolds numbers regime (Garside & Al-Dibouni 1977; Di Felice 1999).

Efficient algorithms and sufficient computational power have become available only relatively recently and since then many different numerical methods have been used to improve our understanding of the problem (Prosperetti 2015). Among others we recall the dynamical simulations performed by Ladd (1993), the finite-elements simulations of Johnson & Tezduyar (1996), the force-coupling method simulations by Climent & Maxey (2003), the Lattice-Boltzmann simulations of Yin & Koch (2007), the Oseenlet simulations by
Sedimentation of finite-size spheres

Pignatel et al. (2011), and the Immersed Boundary simulations of Kempe & Fröhlich (2012) and Uhlmann & Doychev (2014). Thanks to the most recent techniques it has become feasible to gain more insight on the interactions among the different phases and the resulting microstructure of the sedimenting suspension (Yin & Koch 2007; Uhlmann & Doychev 2014). Uhlmann & Doychev (2014), most recently, simulated the settling of dilute suspensions with particle Reynolds numbers in the range $100 - 260$ and studied the effect of the Archimedes number (namely the ratio between gravitational and viscous forces) on the microscopic and macroscopic properties of the suspension. These authors observe an increase of the settling velocity at higher Archimedes, owing to particle clustering in a regime where the flow undergoes a steady bifurcation to an asymmetric wake. Settling in stratified environments has also been investigated experimentally, i.e. by Bush et al. (2003), and numerically, i.e. by Doostmohammadi & Ardekani (2015).

1.2. Sedimentation in an already turbulent flow

The investigations previously reported consider the settling of particles in quiescent or uniform flows. There are many situations though, where the ambient fluid is in fact nonuniform or turbulent. As in the previous case, the first approach to this problem was analytical. In the late 40’s and 50’s Tchen (1947) and later Corrsin & Lumley (1956) proposed an equation for the motion of a small rigid sphere settling in a nonuniform flow. In the derivation, they assumed the particle Reynolds number to be very low so that the viscous Stokes drag for a sphere could be applied. The added mass and the augmented viscous drag due to a Basset history term were also included. Maxey & Riley (1983) corrected these equations including also the Faxen forces due to the unsteady Stokes flow.

In a turbulent flow many different spatial and temporal scales are active. Therefore the behaviour and motion of one single particle does not depend only on its dimensions and characteristic response time, but also on the ratios among these and the characteristic turbulent length and time scales. The turbulent quantities usually considered are the Kolmogorov length and time scales which are related to the smallest eddies. Alternatively, the integral lengthscale and the eddy turnover time can also be used. It is clear that a particle smaller than the Kolmogorov lengthscale will behave differently than a particle of size comparable to the energetic flow structures. A sufficiently large particle with a characteristic time scale larger than the timescale of the velocity fluctuations will definitely be affected by and affect the turbulence. A smaller particle with a shorter relaxation time will more closely follow the turbulent fluctuations. When particle suspensions are considered, the situation becomes even more complicated. If the particles are solid, smaller than the Kolmogorov lengthscale and dilute, the turbulent flow field is unaltered (i.e., one-way coupling). Interestingly, the turbulent dynamics is instead altered by microbubbles. The presence of these microbubbles leads to relevant drag reduction in boundary
layers and shears flows (e.g. Taylor-Couette flow) (Sugiyama et al. 2008; Cecicio 2010). If the mass of the dispersed phase is similar to that of the carrier phase, the influence of the solid phase on the fluid phase cannot be ignored (i.e., two-way coupling). Interactions among particles (such as collisions) must also be considered in concentrated suspensions. This last regime is described as four-way coupling (Elgobashi 1991; Balachandar & Eaton 2010).

Because of the difficulty of treating the problem analytically, the investigations of the last three decades have mostly been either experimental or numerical. In most of the numerical studies heavy and small particles were considered. The reader is referred to Toschi & Bodenschatz (2009) for a more detailed review than the short summary reported here. Wang & Maxey (1993) studied the settling of dilute heavy particles in homogeneous isotropic turbulence. The particle Reynolds number based on the relative velocity was assumed to be much less than unity so that Stokes drag force could be used to determine the particle motion. These authors show that heavy particles smaller than the Kolmogorov lengthscale tend to move outward from the center of eddies and are often swept into regions of downdrafts (the so called preferential sweeping later renamed fast-tracking). In doing so, the particle mean settling velocity is increased with respect to that in a quiescent fluid. A series of studies confirmed and extended these results examining particle clustering (Bec et al. 2014; Gustavsson et al. 2014), preferential concentration (Aliseda et al. 2002), the effects of the particle shape, orientation and collision rates (Siewert et al. 2014), as well the effects of one- or two-way coupling algorithms (Bosse et al. 2006), to mention few aspects. Numerous experimental studies were also performed in order to confirm these results and to study the turbulence modulation due to the presence of particles (Hwang & Eaton 2006).

The results on the mean settling velocities of particles of the order or larger than the Kolmogorov scale are not conclusive. Good et al. (2014) studied particles smaller than the Kolmogorov scale and with density ratio $\mathcal{O}(1000)$, whereas Variano (experiments; private communication) and Byron (2015) studied finite-size particles at density ratios comparable to ours. Good et al. (2014) found that the mean settling velocity is reduced only when nonlinear drag corrections are considered in a one-way coupling approach when particles have a long relaxation time (a linear drag force would always lead to a settling velocity enhancement). For finite-size almost neutrally-buoyant particles, Variano and Byron (2015) observe instead that the mean settling velocity is smaller than in a quiescent fluid. In relative terms, the settling velocity decreases more and more as the ratio between the turbulence fluctuations and the terminal velocity of a single particle in a quiescent fluid increases. It is generally believed that the reduction of settling speed is due to the non-linear relation between the particle drag and the Reynolds number. Nonetheless, unsteady and history effects may also play a key role (Olivieri et al. 2014; Bergougnoux et al. 2014). Tunstall & Houghton (1968) demonstrated already in 1968 that the average settling velocity is reduced in a flow oscillating about a zero mean, due to the interactions.
of the particle inertia with a non-linear drag force. Stout et al. (1995) tried to motivate these findings in terms of the relative motion between the fluid and the particles. When the period of the fluid velocity fluctuations is smaller than the particle response time, a significant relative motion is generated between the two phases. Due to the drag non-linearity, appreciable upward forces can be produced on the particles thereby reducing the mean settling velocity. Unsteady effects may become important when considering suspensions with moderate particle-fluid density ratios, as suggested by Mordant & Pinton (2000) and Sobral, Oliveira & Cunha (2007). The former studied experimentally the motion of a solid sphere settling in a quiescent fluid and explain the transitory oscillations of the settling velocity found at $Re \approx O(100)$ by the presence of a transient vortex shedding in the particle wake. The latter, instead, analyzed an equation similar to that proposed by Maxey & Riley (1983), and suggested that unsteady hydrodynamic drags might become important when the density ratio approaches unity.

1.3. Fully resolved simulations

As already mentioned, most of the numerical studies of settling in turbulent flows used either one or two-way coupling algorithms. In order to properly understand the microscopical phenomena at play, it would be ideal to use fully resolved simulations. An algorithm often used to accomplish this is the Immersed Boundary Method with direct forcing for the simulation of particulate flows originally developed by Uhlmann (2005). The code was later used to study the clustering of non-colloidal particles settling in a quiescent environment (Uhlmann & Doychev 2014). With a similar method Lucci et al. (2010) studied the modulation of isotropic turbulence by particles of Taylor length-scale size. Recently, Homann et al. (2013) used an Immersed Boundary Fourier-spectral method to study finite-size effects on the dynamics of single particles in turbulent flows. These authors found that the drag force on a particle suspended in a turbulent flow increases as a function of the turbulent intensity and the particle Reynolds number. We recently used a similar algorithm to examine turbulent channel flows of particle suspensions (Picano, Breugem & Brandt 2015).

The aim of the present study is to simulate the sedimentation of a suspension of particles larger than the Kolmogorov lengthscale in homogeneous isotropic turbulence with a finite difference Immersed Boundary Method. We focus on particles slightly denser than the suspending fluid ($\rho_p/\rho_f = 1.02$) and investigate particle and fluid velocity statistics, non-linear and unsteady contributions to the overall drag and turbulence modulation. The suspensions considered in this work are dilute ($\phi = 0.5 - 1\%$) and monodispersed. The same simulations are also performed in absence of turbulence to appreciate differences of the particle velocity statistics in the two different environments. Due to the size of the particles considered it has been necessary to consider very long computational domains in the settling direction, especially for the
quiescent environment. In the turbulent cases, smaller domains provide converged statistics since the particle wakes are disrupted faster. The parameters of the simulations have been inspired by the experiments by Variano, Byron (2015) and co-workers at UC Berkeley. These authors investigate Taylor-scale particles in turbulent aquatic environments using Refractive-Index-Matched Hydrogel particles to measure particle linear and angular velocities.

Our results show that the mean settling velocity is lower in an already turbulent flow than in a quiescent fluid. The reduction is about 12% and 14% for the two volume fractions investigated. By looking at probability density functions pdf of the settling velocities, we observe that the pdf is well approximated by a Gaussian function centered around the mean in the turbulent cases. In the laminar case instead, the pdf shows a smaller variance and a larger skewness, indicating that it is more probable to find particles settling more rapidly than the mean value rather than more slowly. These events are associated to particle-particle interactions, in particular to the drifting-kissing-tumbling motion of particle pairs. We also calculate mean relative velocity fields and notice that vortex shedding occurs around each particle in a turbulent environment. Using the concept of mean relative velocity we calculate a local Reynolds number and the mean drag coefficient from empirical formulas to quantify the importance of unsteady and history effects on the overall drag, thereby explaining the reduction in mean settling velocity. In fact, these terms become important only in a turbulent environment.

2. Methodology

2.1. Numerical Algorithm

Different methods have been proposed in the last years to perform Direct Numerical Simulations of multiphase flows. The Lagrangian-Eulerian algorithms are believed to be the most appropriate for solid-fluid suspensions (Ladd & Verberg 2001; Zhang & Prosperetti 2010; Lucci et al. 2010; Uhlmann & Doychev 2014). In the present study, simulations have been performed using a tri-periodic version of the numerical code originally developed by Breugem (2012) that models the coupling between the solid and fluid phases. The Eulerian fluid phase is evolved according to the incompressible Navier-Stokes equations,

$$\nabla \cdot \mathbf{u}_f = 0$$

$$\frac{\partial \mathbf{u}_f}{\partial t} + \mathbf{u}_f \cdot \nabla \mathbf{u}_f = -\frac{1}{\rho_f} \nabla p + \nu \nabla^2 \mathbf{u}_f + \mathbf{f}$$

where $\mathbf{u}_f$, $\rho_f$ and $\nu = \mu/\rho_f$ are the fluid velocity, density and kinematic viscosity respectively ($\mu$ is the dynamic viscosity), while $p$ and $\mathbf{f}$ are the pressure and the force field used to maintain turbulence and model the presence of particles. The particles centroid linear and angular velocities, $\mathbf{u}_p$ and $\mathbf{\omega}_p$ are instead
governed by the Newton-Euler Lagrangian equations,

\[
\rho_p V_p \frac{du_p}{dt} = \rho_f \oint_{\partial V_p} \tau \cdot n \, dS + (\rho_p - \rho_f) V_p g \\
I_p \frac{d\omega_p}{dt} = \rho_f \oint_{\partial V_p} \mathbf{r} \times \tau \cdot n \, dS
\]

where \( V_p = \frac{4}{3} \pi a^3 \) and \( I_p = \frac{2}{5} \rho_p V_p a^5 \) are the particle volume and moment of inertia, with \( a \) the particle radius; \( g \) is the gravitational acceleration; \( \tau = -p I + 2 \mu E \) is the fluid stress, with \( I \) the identity matrix and \( E = \frac{\nabla u_f + \nabla u_f^T}{2} \) the deformation tensor; \( \mathbf{r} \) is the distance vector from the center of the sphere while \( n \) is the unit vector normal to the particle surface \( \partial V_p \). Dirichlet boundary conditions for the fluid phase are enforced on the particle surfaces as \( u_f |_{\partial V_p} = u_p + \omega_p \times \mathbf{r} \).

In the numerical code the coupling between the solid and fluid phases is obtained by using an Immersed Boundary Method. The boundary condition at the moving particle surface (i.e. \( u_f |_{\partial V_p} = u_p + \omega_p \times \mathbf{r} \)) is modeled by adding a force field on the right-hand side of the Navier-Stokes equations. The problem of re-meshing is therefore avoided and the fluid phase is evolved in the whole computational domain using a second order finite difference scheme on a staggered mesh. The time integration is performed by a third order Runge-Kutta scheme combined with a pressure-correction method at each sub-step. The same integration scheme is also used for the Lagrangian evolution of eqs. (4) and (5). The forces exchanged by the fluid and the particles are imposed on \( N_L \) Lagrangian points uniformly distributed on the particle surface. The force \( \mathbf{F}_l \) acting on the \( l \)-th Lagrangian point is related to the Eulerian force field \( \mathbf{f} \) by the expression \( \mathbf{f}(x) = \sum_{l=1}^{N_L} \mathbf{F}_l \delta_d(x - \mathbf{X}_l) \Delta V_l \). In the latter \( \Delta V_l \) represents the volume of the cell containing the \( l \)-th Lagrangian point while \( \delta_d \) is the Dirac delta. This force field is obtained through an iterative algorithm that maintains second order global accuracy in space. Using this IBM force field eqs. (4) and (5) are rearranged as follows to maintain accuracy,

\[
\rho_p V_p \frac{du_p}{dt} = -\rho_f \sum_{l=1}^{N_L} \mathbf{F}_l \Delta V_l + \rho_f \frac{d}{dt} \int_{V_p} u_f \, dV + (\rho_p - \rho_f) V_p g \\
I_p \frac{d\omega_p}{dt} = -\rho_f \sum_{l=1}^{N_L} \mathbf{r}_l \times \mathbf{F}_l \Delta V_l + \rho_f \frac{d}{dt} \int_{V_p} \mathbf{r} \times u_f \, dV
\]

where the second terms on the right-hand sides are corrections to account for the inertia of the fictitious fluid contained within the particle volume. In eqs. (6),(7) \( \mathbf{r}_l \) is simply the distance from the center of a particle. Particle-particle interactions are also considered. When the gap distance between two particles is smaller than twice the mesh size, lubrication models based on Brenner’s asymptotic solution (Brenner 1961) are used to correctly reproduce the interaction between the particles. A soft-collision model is used to account for
collisions among particles with an almost elastic rebound (the restitution coefficient is 0.97). These lubrication and collision forces are added to the right-hand side of eq. (6). More details and validations of the numerical code can be found in Breugem (2012), Lambert et al. (2013), Lashgari et al. (2014) and Picano et al. (2015).

2.2. Parameter setting

Sedimentation of dilute particle suspensions is considered in an unbounded computational domain with periodic boundary conditions in the $x$, $y$ and $z$ directions. Gravity is chosen to act in the positive $z$ direction. A zero mass flux is imposed in the simulations. A cubic mesh is used to discretise the computational domain with eight points per particle radius, $a$. Non-Brownian rigid spheres are considered with solid to fluid density ratio $\rho_p/\rho_f = 1.02$. Hence, we consider particles slightly heavier than the suspending fluid. Two different solid volume fractions $\phi = 0.5\%$ and $1\%$ are considered. In addition to the solid to fluid density ratio $\rho_p/\rho_f$ and the solid volume fraction $\phi$, it is necessary to introduce another nondimensional number. This is the Archimedes number (or alternatively the Galileo number $Ga = \sqrt{Ar}$),

$$Ar = \frac{\left(\frac{\rho_p}{\rho_f} - 1\right)g(2a)^3}{\nu^2} \quad (7)$$

a nondimensional number that quantifies the importance of the gravitational forces acting on the particle with respect to viscous forces. In the present case the Archimedes number $Ar = 21000$. Using the particle terminal velocity $v_t$ we define the Reynolds number $Re_t = 2av_t/\nu$. This can be related by empirical relations to the drag coefficient of an isolated sphere when varying the Archimedes number, $Ar$. Different versions of these empirical relations giving the drag coefficient as a function of $Re_t$ and $Ar$ have been proposed. As Yin & Koch (2007) we will use the following relations,

$$C_D = \left\{ \begin{array}{ll}
\frac{24}{Re_t} \left[ 1 + 0.1315 Re_t^{0.82 - 0.05 \log_{10} Re_t} \right], & 0.01 < Re_t \leq 20 \\
\frac{24}{Re_t} \left[ 1 + 0.1935 Re_t^{0.6305} \right], & 20 < Re_t < 260
\end{array} \right. \quad (8)$$

since $C_D = 4Ar/(3Re_t^2)$ (Yin & Koch 2007) we finally write,

$$Ar = \left\{ \begin{array}{ll}
18Re_t \left[ 1 + 0.1315 Re_t^{0.82 - 0.05 \log_{10} Re_t} \right], & 0.01 < Re_t \leq 20 \\
18Re_t \left[ 1 + 0.1935 Re_t^{0.6305} \right], & 20 < Re_t < 260
\end{array} \right. \quad (9)$$

The Reynolds number calculated from eq. (9) is approximately 188 for $Ar = 21000$. In order to generate and sustain an isotropic and homogeneous turbulent flow field, a random forcing is applied to the first shell of wave vectors. We consider a $\delta$-correlated in time forcing of fixed amplitude $\hat{f}_0$ (Vincent & Meneguzzi 1991; Zhan et al. 2014). The turbulent field, alone, is characterized by a Reynolds number based on the Taylor microscale, $Re_\lambda = \lambda u'/\nu$, where $u'$ is the fluctuating velocity and $\lambda = \sqrt{15\nu u'^2/\epsilon}$ is the transverse Taylor length scale.
Sedimentation of finite-size spheres

Figure 1. Terminal velocity of a periodic array of spheres. Present results \( Re_t = 1 \) denoted by red circles are compared with the ones obtained by Yin and Koch by black squares at the same \( Re_t \) and with the analytical solution for \( Re_t = 0 \) of eq. (10).

This is about 90 in our simulations. The ratio between the grid spacing and the Kolmogorov lengthscale \( \eta = (\nu^3/\epsilon)^{1/4} \) (where \( \epsilon \) is the energy dissipation) is approximately 1.3 while the particle diameter is circa 12\( \eta \). Finally, the ratio among the expected mean settling velocity and the turbulent velocity fluctuations is \( v_t/u' = 3.4 \). The parameters of the turbulent flow field are summarized in table 1. For the definition of these parameters, the reader is referred to Pope (2000).

2.3. Validation

To check the validity of our approach we performed simulations of a single sphere settling in a cubic lattice in boxes of different sizes. Since this is equivalent to changing the solid volume fraction, we compared our results to the analytical formula derived by Hasimoto (1959) and Sangani & Acrivos (1982),

\[
|V_t| = \left| \frac{V_t}{V_s} \right| = 1 - 1.7601 \phi^{1/3}
\]

where

\[
|V_s| = \frac{2}{9} \left( \frac{\rho_p - 1}{\rho_f} \right) g a^2 \nu
\]

is the Stokes settling velocity. In terms of the size of the computational domain, \( l_z \), eq. (10) can also be rewritten as \( V_t = 1 - 1.7601(2a/l_z)(\pi/6)^{1/3} \). In figure 1 we show the results obtained with our code for \( Re_t = 1 \) together with the data by Yin & Koch (2007) and the analytical solution. Although the analytical solution was derived with the assumption of vanishing Reynolds numbers, we find good agreement among the various results.

The actual problem arises when considering particles settling at relatively high Reynolds numbers. If the computational box is not sufficiently long in
the gravity direction, a particle would fall inside its own wake (due to periodic boundary conditions), thereby accelerating unrealistically. Various simulations of a single particle falling in boxes of different size were preliminarily carried out, in particular $48a \times 48a \times 48a$, $32a \times 32a \times 96a$ and $32a \times 32a \times 320a$. The first two boxes turn out to be unsuitable for our purposes. We find a terminal Reynolds number $Re_t = 200$ in the longest domain considered, which corresponds to a difference of about 6% with respect to the value obtained from the empirical relations (9). As reference velocity we use the value obtained from simulations performed in the largest box at a solid volume fraction two orders of magnitude smaller than the cases under investigation, $\phi = 5 \cdot 10^{-5}$ (as in Uhlmann & Doychev 2014), corresponding to a terminal velocity such that $Re_t = 195$, 4% larger than the value from the empirical relations (9). Further increasing the length in the $z$ direction would make the simulations prohibitive. Note also that simulations in a turbulent environment turn out to be less demanding as turbulence disrupts and decorrelates the flow structures induced by the particles. The final choice was therefore a computational box of size $32a \times 32a \times 320a$ with $256 \times 256 \times 2560$ grid points, 391 particles for $\phi = 0.5\%$ and 782 particles for $\phi = 1\%$. In all cases, the particles are initially distributed randomly in the computational volume with zero initial velocity and rotation.

A snapshot of the suspension flow for $\phi = 0.5\%$ is shown in figure 2. The instantaneous velocity component perpendicular to gravity is shown on different orthogonal planes.

The simulations were run on a Cray XE6 system at the PDC Center for High Performance Computing at the KTH, Royal Institute of Technology. The fluid phase is evolved for approximately 6 eddy turnover times before adding the solid phase. The simulations for each solid volume fraction were performed for both quiescent fluid and turbulent flow cases in order to compare the results. Statistics are collected after an initial transient phase of about 4 eddy turnover times for the turbulent case and 15 relaxation times ($T_p = 2\rho_p a^2/(9\rho_f \nu)$) for the quiescent case. Defining as reference time the time it takes for an isolated particle to fall over a distance equal to its diameter, $2a/v_t$, the initial transient corresponds to approximately 170 units. Statistics are collected over a time interval of 500 and 300 in units of $2a/v_t$ for the quiescent and turbulent cases, respectively. Differences between the statistics presented here and those computed from half the samples is below 1% for the first and second moments.
3. Results

We investigate and compare the behavior of a suspension of buoyant particles in a quiescent and turbulent environment. The behaviour of a suspension in a turbulent flow depends on both the particles and turbulence characteristic time- and length-scales: homogeneous and isotropic turbulence is defined by the dissipative, Taylor and integral scales, whereas the particles are characterized by their settling velocity $v_t$ and by their Stokesian relaxation time $T_p = 2\rho_p a^2/(9\rho_f \nu) = 11.1$ (time is scaled by $(2a/v_t)$ throughout the paper). A comparison between characteristic time scales is given by the Stokes number, i.e. the ratio between the particle relaxation time and a typical flow time scale $St_f = T_p/T_f$. In the present cases, the Stokes number based on the dissipative scales (time and velocity) is $St_\eta = T_p/T_K = 8.1$ so the particles are inertial on this scale. In addition, because the particles are about 12 times larger than the Kolmogorov length and fall about 16 times faster than the Kolmogorov velocity scale, we can expect that motions at the smallest scales weakly affect the particle dynamics.

Considering therefore the large-scale motions, we introduce an integral-scale Stokes number $St_{Te} = T_p/T_e = 0.24$. This value of $St_{Te}$ reflects the fact that the particles are about 20 times smaller than the integral length scale $L_0$. The strong coupling between particle dynamics and turbulent flow field occurs at scales of the order of the Taylor scale for the present cases. Indeed, the Taylor Stokes number is $St_\lambda = T_p/T_\lambda = 2.1$ with $T_\lambda = \lambda/u'$. It should be noted that the Taylor length is slightly larger than the particle size, $3.1a$, while
3.1. Particle statistics

We start by comparing the single-point flow and particle velocity statistics for the two cases studied, i.e. quiescent and turbulent flow. The results are collected when a statistically steady state is reached. Due to the axial symmetry with respect to the direction of gravity, we consider only two velocity components for both phases, the components parallel and perpendicular to gravity, $V_{p,\tau}$ and $V_{p,n}$ respectively, where $\alpha = f, p$ indicates the solid and fluid phases.

In figure 3 we report the probability density function of the particle velocities for both volume fraction investigated here, $\phi = 0.5\%$ and 1%; the moments extracted from these distribution are summarized in table 2. The data in 3a) show the pdf for the component of the velocity aligned with gravity $V_{p,\tau}$ normalized by the settling velocity for $\phi \to 0$ in a quiescent environment, $v_t$. This is extracted from the simulation of a very dilute suspension discussed in section 2.3.

In the quiescent cases, the mean settling velocity slightly reduces when increasing the volume fraction $\phi$, in agreement with the findings of Richardson & Zaki (1954) and Di Felice (1999) among others. The sedimentation velocity decreases to 0.96 at $\phi = 0.5\%$ and 0.93 at $\phi = 1\%$. Di Felice (1999) investigated experimentally the settling velocity of dilute suspensions of spheres ($\phi = 0.5\%$)
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with density ratio 1.2 in quiescent fluid, for a large range of terminal Reynolds numbers (from 0.01 to 1000). Following the empirical fit proposed in Di Felice (1999), we obtain \( \langle V_{f,\tau} \rangle \approx 0.98 \) at \( \phi = 0.5\% \), approximately 1% larger than our result. On the other hand, the formula suggested for the intermediate regime in Di Felice (1999) and Yin & Koch (2007), \( Re_t < 150 \), would give an estimated value of 0.88, 6% lower than our result.

The mean settling velocity for the quiescent case at \( \phi = 0.5\% \) is instead close to the estimated value from eq. (9). This is in agreement with what reported in Uhlmann & Doychev (2014). These authors found that the particle mean settling velocity of a dilute suspension increases above the reference value only when the Archimedes number \( Ar \) is larger than approximately 24000 and clustering occurs. In our case \( Ar \approx 21000 \) and no clustering is noticed accordingly with their findings.

Interestingly, we observe an additional non-negligible reduction when a turbulent background flow is considered, in our opinion the main result of the paper. The reduction of the mean settling velocity \( \langle V_{p,\tau} \rangle \) is 12% at \( \phi = 0.5\% \) and 14% at \( \phi = 1\% \), see table 2. This result unequivocally shows that the turbulence reduces the settling velocity of a suspension of finite-size buoyant particles, in agreement with the experimental findings by Variano and co-workers (Variano, private communication) and Byron (2015). We also note that the reduction of the settling velocity with the volume fraction is less important for the turbulent cases.

Looking more carefully at the pdfs we note that fluctuations are, as expected, larger in a turbulent environment. In addition, the vertical particle velocity fluctuations are the largest component in a quiescent fluid, whereas in a turbulent flow the fluctuations are largest in the horizontal directions, as summarized in table 2. In the quiescent case the rms of the tangential velocity \( \sigma_{V_p,\tau} \) is 0.15 and 0.17 for \( \phi = 0.5\% \) and \( \phi = 1\% \) respectively, while it increases up to 0.23 in the corresponding turbulent cases. The difference in the width of the pdf is particularly large in the directions normal to gravity where the rms of the variance \( \sigma_{V_p,n} \) is 0.3 for both turbulent cases, while it is 5 and 4 times smaller for the quiescent flows at \( \phi = 0.5\% \) and \( \phi = 1\% \). We believe that the interactions among the particle wakes, mainly occurring in the settling direction, promote the higher vertical velocity fluctuations found in the quiescent cases. The shape of the pdf is essentially Gaussian for the turbulent cases, showing vanishing skewness and normal flatness. Interestingly an intermittent and skewed behaviour is exhibited in the quiescent cases. The flatness \( K \) is around 9 for both components at \( \phi = 0.5\% \) and slightly reduces to 5.5 at \( \phi = 1\% \). The settling velocity of the quiescent cases is skewed towards intense fluctuations in the direction of the gravity. The skewness \( S \) is higher for the more dilute case, being 1.26 at \( \phi = 0.5\% \) and 0.7 at \( \phi = 1\% \).

We interpret the intermittent behavior suggested by values of \( K > 3 \) by the collective dynamics of the particle suspension. The significant tails of the pdfs shown in figure 3a) are indeed associated to a specific behavior: as particles
fall, they tend to be accelerated by the wakes of other particles, before showing drafting-kissing-tumbling behavior (Fortes et al. 1987). Snapshots of the drafting-kissing-tumbling behavior between two spherical particles are shown in figure 4. When this close interaction occurs, particles are found to fall with velocities that can be more than twice the mean settling velocity $\langle V_{p,\tau} \rangle$. In the quiescent case the fluid is still, the wakes are the only perturbation present in the field and are long and intense so their effect can be felt far away from the reference particle. The more dilute the suspension the more intermittent the particle velocities are. On the contrary, when the flow is turbulent the wakes are disrupted quickly and therefore fewer particles feel the presence of a wake. The velocity disturbances are now mainly due to turbulent eddies of different size that interact with the particles to increase the variance of the velocity homogeneously along all directions leading to the almost perfect normal distributions shown above, with variances similar to those of the turbulent fluctuations. The features of the particle wakes will be further discussed in this manuscript to support the present explanation.

We also note that the sedimenting speed in the quiescent fluid is determined by two opposite contributions. The excluded volume effect that contributes to a reduction of the mean settling velocity with respect to an isolated sphere and the pairwise interactions (the drafting-kissing-tumbling), increasing the mean velocity of the two particles involved in the encounter. To try to identify the importance of the drafting-kissing-tumbling effect, we fit the left part (where no intermittent behaviour is found) of the pdf pertaining the quiescent case at $\phi = 0.5\%$ with a gaussian function. The mean of $V_{p,\tau}$ is reduced to about 0.93 (value due only to the hindrance effect) instead of 0.96 in the full simulation; thereby the increment in mean settling velocity due to drafting-kissing-tumbling can be estimated to be of about 3%.

|                  | Quiescent $\phi = 0.5\%$ | Turbulent $\phi = 0.5\%$ | Quiescent $\phi = 1\%$ | Turbulent $\phi = 1\%$
|------------------|--------------------------|--------------------------|--------------------------|--------------------------
| $\langle V_{p,\tau} \rangle$ | +0.96                    | +0.88                    | +0.93                    | +0.86                    |
| $\sigma_{V_{p,\tau}}$ | +0.15                    | +0.23                    | +0.17                    | +0.23                    |
| $S_{V_{p,\tau}}$ | +1.26                    | +0.01                    | +0.70                    | +0.01                    |
| $K_{V_{p,\tau}}$ | +9.65                    | +2.92                    | +6.01                    | +3.15                    |

$\langle V_{p,n} \rangle$ $+0.33 \cdot 10^{-4}$ $-1.93 \cdot 10^{-3}$ $-8.78 \cdot 10^{-4}$ $-0.97 \cdot 10^{-3}$
$\sigma_{V_{p,n}}$ $+0.06$ $+0.31$ $+0.08$ $+0.31$
$S_{V_{p,n}}$ $-1.22 \cdot 10^{-3}$ $+0.04$ $-3.17 \cdot 10^{-3}$ $+0.07$
$K_{V_{p,n}}$ $+8.95$ $+2.78$ $+5.55$ $+2.80$

Table 2. First four central moments of the probability density functions of $V_{p,\tau}$ and $V_{p,n}$ normalized by $v_t$. $S_{V_{p,\tau}}$ ($S_{V_{p,n}}$) and $K_{V_{p,\tau}}$ ($K_{V_{p,n}}$) are respectively the skewness and the flatness of the pdf’s.
Figure 4. Drafting-kissing-tumbling behavior among two spherical particles in the quiescent case with \( \phi = 0.5\% \). The particles are coloured with the absolute value of their velocity component in the direction of gravity. Three particles are labeled with ”A,B,C” in order to show how accelerated the two interacting particles are compared to the others.

The probability density function of the particle angular velocities are also different in quiescent and turbulent flows. These are shown in figures 5a) and b) for rotations about an axis parallel to gravity, \( |\omega_{p,\tau}| = |\omega_{p,z}| \), and
Figure 5. Probability density functions of a) $|\omega_{p,z}|$ and b) $\sqrt{\omega_{p,x}^2 + \omega_{p,y}^2}$ for $\phi = 0.5\%$ and $1\%$. The angular velocities are normalized by $v_t/(2a)$, the settling velocity of a single particle in a quiescent environment and its diameter. Quiescent fluid cases denoted by blue curve with squares for $\phi = 0.5\%$ and green curve with triangles for $\phi = 1\%$, turbulent flow data by red curve with circles for $\phi = 0.5\%$ and black curve with downward-pointing triangles for $\phi = 1\%$.

Orthogonal to it, $\sqrt{\omega_{p,x}^2 + \omega_{p,y}^2}$. In the settling direction the peak of the pdf is always at $|\omega_{p,z}| = 0$. As for the translational velocities, the pdfs are broader in the turbulent cases. Due to the interaction with turbulent eddies, particles tend also to spin faster around axis perpendicular to gravity. From figure 5b) we see that the modal value slightly increases in the quiescent cases when increasing the volume fraction. In the turbulent cases, the modal value is more than 3 times the values of the quiescent cases and the variance is also increased. Unlike the quiescent cases, the curves almost perfectly overlap for the two different $\phi$, meaning that turbulent fluctuations dominate the particle dynamics. Turbulence hinders particle hydrodynamic interactions.

Figure 6 shows the temporal correlations of the particle velocity fluctuations,

$$R_{v,v}(\Delta t) = \frac{\langle V'_{p,\tau}(p,t)V'_{p,\tau}(p,t+\Delta t)\rangle}{\sigma_{V_p,\tau}^2}$$  \hspace{1cm} (12)

$$R_{v,v}(\Delta t) = \frac{\langle V'_{p,n}(p,t)V'_{p,n}(p,t+\Delta t)\rangle}{\sigma_{V_p,n}^2}$$  \hspace{1cm} (13)

for the turbulent and quiescent cases at $\phi = 0.5\%$ and $\phi = 1\%$. Focusing on the data at the lower volume fraction, we observe that the particle settling velocity decorrelates much faster in the turbulent environment, within $\Delta t \sim 50$, while it takes around one order of magnitude longer in a quiescent fluid. Falling particles may encounter intense vortical structures that change their settling
velocity. The turbulence strongly alters the fluid velocity field seen by the particles, which in the quiescent environment is only constituted by coherent long particle wakes. This results in a faster decorrelation of the velocity fluctuations along the settling direction in the turbulent environment. Moreover, $R_{v_n v_n}$ crosses the null value earlier than for the settling velocity component. This result is not surprising since the particle wakes develop only in the settling direction.

The normal velocity correlation $R_{v_n v_n}$ of the turbulent case oscillates around zero before vanishing at longer times. We attribute this to the presence of the large-scale turbulent eddies. As a settling particle encounters sufficiently strong and large eddies, its trajectory is swept on planes normal to gravity in an oscillatory way. To provide an approximate estimate of this effect, we consider as a first approximation the turbulent flow seen by the particles as frozen since the particles fall at a higher velocity than the turbulent fluctuations (3.4 times). Since the strongest eddies are of the order of the transversal integral scale we can presume that these structures are responsible for this behavior. In particular, the transversal integral scale $L_T = L_0/2 \simeq 8$ and $u'_{rms} = 0.3$, 

**Figure 6.** Time correlations of the particle velocity fluctuations. The blue curve with circles represents the correlation of $V'_{p,\tau} (R_{v, v})$, while the red curve with diamonds is used for the correlation of $V'_{p,n} (R_{v_n, v_n})$. a) Quiescent case with $\phi = 0.5\%$, b) Turbulent case with $\phi = 0.5\%$, c) Quiescent case with $\phi = 1.0\%$ and d) Turbulent case with $\phi = 1.0\%$. 
we expect a typical period of $t = L_T/u'_{rms} \simeq 26$ which is of the order of the oscillations found for both turbulent cases, i.e. $t \approx 20$. Note that a similar behavior has been observed by Wang & Maxey (1993) for sufficiently small and heavy particles, termed the preferential sweeping phenomenon.

The same process can be interpreted in terms of crossing trajectories and continuity effects as described by Csanady (1963). An inertial particle falling in a turbulent environment changes continuously its fluid-particle neighborhood. It will fall out from the eddy where it was at an earlier instant and will therefore rapidly decorrelate from the flow. In order to accommodate the back-flow necessary to satisfy continuity, the normal correlations must then contain negative loops (as those seen in figures 6b and d). Following Csanady (1963) we define the period of oscillation of the fluctuations as the ratio of the typical eddy diameter in the direction of gravity (i.e. the longitudinal integral scale $L_0$), and the particle terminal velocity $v_t$ obtaining $t = L_0/v_t \simeq 16$. This value is similar to the period of oscillations in the correlations in figure 6.

As shown in figure 6c), the quiescent environment presents a peculiar behavior of the settling velocity correlation at $\phi = 1\%$. In particular we observe oscillations around zero of long period, $T = 160 – 180$. From the analysis of particle snapshots at different times (not shown), we observe that these seem correlated to the formation of regions of different density of the particle concentration. Hence a particle crossing regions with different local particle concentration may experience a varying settling velocity.

To further understand the particle dynamics, we display in figure 7a) and b) the single particle dispersion, i.e. the mean square displacement, for both quiescent and turbulent cases at $\phi = 0.5\%$ and $1.0\%$. The mean displacement, $\langle V_p, \tau \rangle$, is subtracted from the instantaneous displacement in the settling direction $\Delta z(t)$ to highlight the fluctuations with respect to the mean motion. For all cases we found initially a quadratic scaling in time ($\langle \Delta z^2 \rangle \sim t^2$) typical of correlated motions while the linear diffusive behavior takes over at longer times ($\langle \Delta z^2 \rangle \sim 2D_e t$ with $D_e$ the diffusion coefficient).

The turbulent cases show a similar behavior for both volume fractions. The crossover time when the initial quadratic scaling is lost and the linear one takes place is about $t \simeq 10$ and $t \simeq 50$ for the normal and tangential component, respectively. This difference is consistent with the correlation timescales previously discussed. The dispersion rates are similar in all directions in a turbulent environment. The quiescent cases present different features. First of all, dispersion is much more effective in the settling direction than in the normal one. The dispersion rate is smaller than the turbulent cases in the horizontal directions, while, surprisingly, the mean square displacement in the settling direction is similar to that of the turbulent cases being even higher at $\phi = 0.5\%$, something we relate to the drafting-kissing-tumbling behaviour discussed above. The crossover time scale is similar to that of turbulent cases with the exception of the most dilute case which does not reach a fully diffusive behavior at $t \simeq 500$. This long correlation time makes the mean square
Figure 7. Mean square particle displacement in the directions parallel and perpendicular to gravity for both quiescent and turbulent cases for a) φ = 0.5% and b) φ = 1%. The mean particle displacement $\langle V_{p,τ} \rangle t$ in the settling direction is subtracted from the instantaneous displacement when computing the statistics. In the inset, we show $\langle \Delta x_i^2 \rangle / t$ as a function of time as well as the diffusion coefficients $D_e$ for the turbulent cases.

Displacement of this case higher than the corresponding turbulent case at long times.

In the insets of figure 7a) and b) we show $\langle \Delta x_i^2 \rangle / t$ as a function of time. In all cases except the quiescent one at φ = 0.5%, the diffusive regime is reached and
it is possible to calculate the diffusion coefficients $D_e = \langle \Delta x_i^2 \rangle / (2t)$. For the turbulent case with $\phi = 0.5\%$ we obtain $D_e = 0.52$ and 0.28 in the directions parallel and perpendicular to gravity while for $\phi = 1\%$ we obtain $D_e = 0.57$ and 0.32. In the quiescent cases the diffusion coefficients in the horizontal directions are approximately 0.03, whereas the coefficient in the gravity direction at $\phi = 1\%$ is about 0.40. Csanady (1963) proposed a theoretical estimate of the diffusion coefficients for pointwise particles. Using these estimates, we obtain approximately $D_e = 1.4$ and 0.7 in the directions parallel and perpendicular to gravity. These are about 2.5 times larger than those found here for finite-size particles.

### 3.2. Fluid statistics

Table 3 reports the fluctuation intensities of the fluid velocities for all cases considered. These are calculated by excluding the volume occupied by the spheres at each time step and averaging over the number of samples associated with the fluid phase volume. As expected, the fluid velocity fluctuations are smaller in the quiescent cases than in the turbulent regime. In the quiescent case the rms of the velocity fluctuations is about 50% larger in the settling direction than in the normal direction because of the long range disturbance induced by the particles wakes. The increase of the volume fraction enhances the fluctuations in both directions. Fluctuations are always larger in the turbulent case, with the most significant differences compared to the quiescent cases in the normal direction, where the presence of the buoyant solid phase brakes the isotropy of the turbulent velocity fluctuations.

Hence, the solid phase clearly affects the turbulent flow field. Although the present study focuses on the settling dynamics, it is interesting to briefly discuss how turbulence is modulated. Modulation of isotropic turbulence by neutrally buoyant particles is examined in Lucci et al. (2010); however the results change due to buoyancy as investigated here. Typical turbulent quantities are reported in table 4 where they are compared with the unladen case at $\phi = 0$. The energy dissipation $\epsilon$ increases with $\phi$ becoming almost double at $\phi = 1\%$. This behavior is expected since the buoyant particles inject energy in the system that is transformed into kinetic energy of the fluid phase that has to be dissipated. The higher energy flux, i.e. dissipation, is reflected in a
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\[ \phi \eta/(2a) \quad k \quad \lambda/(2a) \quad Re_\lambda \quad \epsilon \quad T_\epsilon \quad Re_{L_0} \]

\[
\begin{array}{cccccccc}
0.000 & 0.084 & 0.13 & 1.56 & 90 & 0.0026 & 47.86 & 1205 \\
0.005 & 0.077 & 0.10 & 1.19 & 62 & 0.0037 & 27.97 & 570 \\
0.010 & 0.069 & 0.11 & 1.01 & 54 & 0.0055 & 19.88 & 435 \\
\end{array}
\]

Table 4. Turbulent flow parameters in particle units for $\phi = 0$, $\phi = 0.5\%$ and $\phi = 1\%$.

Reduction of the Kolmogorov length $\eta$. The particles reduce the velocity fluctuations, decreasing the turbulent kinetic energy level. The combined effect on $k$ and $\epsilon$ result in a decrease of the Taylor microscale $\lambda$ and of $Re_\lambda$; likewise the integral length $L_0$ and $Re_{L_0}$ also decrease. The reduction of the large and small turbulence scales is associated to the additional energy injection from the settling particles. Energy injection occurs at the size of the particles, which is below the unperturbed integral scale $L_0$ explaining the lowering of the effective integral $L_0$ and of Taylor $\lambda$ length-scales. This additional energy is transferred to the bulk flow in the particle wake. Associated to this energy input there is a new mechanism for dissipation that is the interaction of the flow with the no-slip surface of the particles. The mean energy dissipation field in the particle reference frame for the turbulent case with $\phi = 0.5\%$ is therefore shown in figure 8. After a statistically steady state is reached, the norm of the symmetric part of the velocity gradient tensor $E_{ij}$ and the dissipation $\epsilon = 2\nu E_{ij}E_{ij}$ are calculated at each time step on a cubic mesh centered around each particle; the dissipation is calculated on the grid points outside the particle volume. The data presented have been averaged over all particles and time to get the mean dissipation field displayed in the figure. The maximum $\langle \epsilon \rangle$ is found around the particle surface with maximum values in the front; the mean dissipation drops down to the values found in the rest of the domain on the particle rear. The overall energy dissipation is therefore made up of two parts: the first associated to the dissipative eddies far from the particle surfaces and the second associated to the mean and fluctuating flow field near the particle surface. To conclude, the settling strongly alters the typical turbulence features via an anisotropic energy injection and dissipation, thus breaking the isotropy of the unladen turbulent flow. The energy is injected by the fluctuations in the particle wake whereas stronger energy dissipation occurs in the front of each particle. As a consequence, the fluid velocity fluctuations change in the directions parallel and perpendicular to gravity as shown in table 3.

3.3. Relative velocity

An important quantity to understand and model the settling dynamics is the particle to fluid relative motion. Although it is still unclear how to properly calculate the slip velocity between the two phases, we consider spherical shells around each particle, centered on the particles centroids, inspired by the works of Bellani & Variano (2012) and Cisse et al. (2013). We calculate the mean
difference between the particle and fluid velocities in each shell as
\[
\langle U_{rel}\rangle_{x,t,NP} = \left\langle u_p - \frac{1}{\Omega(\Delta)} \int_{\Omega(\Delta)} u_f dV \right\rangle_{t,NP}
\]
where \(\Omega(\Delta)\) is the volume of a shell of inner radius \(\Delta\). A parametric study on the slip velocity is performed by changing the inner radii of these spherical shells from \(\Delta = 0.75\) particle diameters to \(\Delta = 5.0\) particle diameters, while keeping the shell thickness \(\delta\) constant and equal to 0.063 in units of \(2a\). In figure 9 we report the component of \(U_{rel}\) parallel to gravity as a function of the shells inner radii \(\Delta/(2a)\). As the shell inner radii increase, \(|U_{rel,\tau}|\) tends exponentially to an
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\[ \Delta/(2a) \quad \langle U_{rel,\tau} \rangle \quad \sigma_{U_{rel,\tau}} \quad S_{U_{rel,\tau}} \quad K_{U_{rel,\tau}} \]

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<th>( \Delta/(2a) )</th>
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<th>( \sigma_{U_{rel,\tau}} )</th>
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Table 5. Moments of the pdf\( (U_{rel,\tau}) \) for \( \phi = 0.5\% \) in the quiescent case. The thickness of the shell used to compute the slip velocity is \( \delta/(2a) = 0.063 \).

\[ \Delta/(2a) \quad \langle U_{rel,\tau} \rangle \quad \sigma_{U_{rel,\tau}} \quad S_{U_{rel,\tau}} \quad K_{U_{rel,\tau}} \]

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<th>( \Delta/(2a) )</th>
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<th>( S_{U_{rel,\tau}} )</th>
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<td>3.10</td>
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Table 6. Moments of the pdf\( (U_{rel,\tau}) \) for \( \phi = 0.5\% \) in a turbulent environment. The thickness of the shell used to compute the slip velocity is \( \delta/(2a) = 0.063 \).

Asymptotic value which corresponds to the mean particle velocity in the same direction, \( \langle V_p,\tau \rangle \). This is expected since the correlation between the fluid and particle velocity goes to zero at large distances. The quiescent cases still show a 0.5% difference between \( |U_{rel,\tau}| \) and \( \langle V_p,\tau \rangle \) at \( \Delta/(2a) = 5 \). This difference is again attributed to the long coherent wakes of the particles.

The probability density function of these relative velocities, \( U_{rel,\tau} \), and their first four central moments are computed and reported in tables 5 and 6 as a function of \( \Delta/(2a) \) for the quiescent fluid and turbulent cases at \( \phi = 0.5\% \). In the turbulent case, the moments approach those of a Gaussian distribution with vanishing skewness and flatness close to 3, especially at large \( \Delta \). In the quiescent case, the third and fourth moments display higher values that decrease as \( \Delta \) is increased, tending to the values of the particle velocities. The pdfs pertaining the four cases considered, calculated in spherical shells with an inner radius of 1.5 and 2.5 particle diameters, are compared in figure 10. A second axis, reporting the the particle Reynolds number \( Re_p \) based on \( U_{rel,\tau} \), is also displayed in each figure. In the former case, \( \Delta/(2a) = 1.5 \), the shell radius is of the order of the Taylor scale to highlight the particle dynamics, while the
relative velocity is approaching the asymptotic values for the larger shell. The pdfs of the relative velocity appear narrower than those of the particle absolute velocity, indicating that the particles tend to be transported by the large-scale motions, filtering the smallest scales.

The distributions pertaining the simulations in a turbulent environment are nearly Gaussian with modal values well below one. The quiescent cases show skewed distributions with long tails at high velocities, as observed for the particle velocities in figure 3a). The particles settle on average with a velocity close to that of a single particle, with occasional events of higher velocity due to the drafting-kissing-tumbling dynamics. The lower the volume fraction the more intermittent is the dynamics.

Knowing the tangential fluid velocity $\langle V_{f,\tau} \rangle_r(p,t)$, averaged in each shell and at each time step, and the corresponding tangential particle velocities $V_{p,\tau}(p,t)$, it is then possible to find their joint probability distribution $P(V_{f,\tau},V_{p,\tau})$ (for sake of simplicity we write $\langle V_{f,\tau} \rangle_r$ as $V_{f,\tau}$). These are evaluated in shells at $\Delta/(2a) = 1.75$ for each case studied and reported in figure 11. In each case, the integral of $P(V_{f,\tau},V_{p,\tau})$,

$$\langle V_{p,\tau}|V_{f,\tau} \rangle = \int_{-\infty}^{\infty} P(V_{f,\tau},V_{p,\tau})V_{f,\tau} dV_{f,\tau},$$  \hspace{1cm} (14)

is also reported (continuous lines). This represents the most probable particle velocity $V_{p,\tau}$ given a certain fluid velocity $V_{f,\tau}$, or, equivalently, the most probable fluid velocity surrounding a particle settling with velocity $V_{p,\tau}$. In the turbulent cases these integrals are well approximated by straight lines (displayed with dashed lines in the figure)

$$V_{p,\tau} = C_1V_{f,\tau} + C_2.$$  \hspace{1cm} (15)
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Figure 11. Joint probability distributions of $V_{f,\tau}$ and $V_{p,\tau}$ evaluated in spherical shells located at 1.75 particle diameters from each particle. We report in panels a) and c) the quiescent cases for $\phi = 0.5\%$ and $1\%$, while the respective turbulent cases are reported in panels b) and d). The continuous lines represent the integrals of the joint probability distributions. In the turbulent cases the dashed lines represent the best-fit of these integrals.

In both cases $C_1$ is approximately 1 while $C_2$ is about 0.86 for $\phi = 0.5\%$ and 0.84 for $\phi = 1\%$. These values are in agreement with the values found for the average relative velocities of shells at $\Delta/(2a) = 1.75$. In a quiescent flow, conversely, the integral in eq. (14) gives a curved line and no best-fit is therefore reported. In these cases, the joint probability distribution is broader, particularly in the region of higher particle velocities, $V_{p,\tau}$. This is again due to the intense particle interactions and the drafting-kissing-tumbling behaviour described in figure 4, which confirms the high flatness of the probability density functions of the relative particle velocities.

Further insight can be obtained by plotting isocontours of the average particle relative velocities and their fluctuations, in both quiescent and turbulent flows. To this end, we follow the approach by Garcia-Villalba et al. (2012). We place an uniform and structured rectangular mesh around each particle, with
origin at the particle center. By means of trilinear interpolations we find the fluid and relative velocities on this local mesh and average over time and the number of particles to obtain the mean relative velocity field and its fluctuations.

The vertical velocity of the single sphere settling in a quiescent fluid is reported in figure 12. The relative normal and tangential velocities and their fluctuations are instead displayed in figure 13 for suspensions with \( \phi = 0.5\% \) in both quiescent and turbulent environment. In the quiescent fluid simulations, a long wake forms behind the representative particle and, as seen from the single point particle velocity correlations, it takes a long time for this velocity fluctuations to decorrelate. In the turbulent case instead, the wakes are disrupted by the background fluctuations.

Interesting observations can be drawn from the relative velocity fluctuation fields. Comparing figures 13c) and 13d) we note that intense vortex shedding occurs around the particles in the turbulent case, with important fluctuations of \( U_{rel,\tau} \). From figures 13e) and 13f) we also see that the relative velocity fluctuations are drastically increased in the horizontal directions in a turbulent environment. Noteworthy, vortex shedding occurs at particle Reynolds numbers below the critical value above which this is usually observed (Bouchet et al. 2006). Vortex shedding is unsteady in nature and unsteady effects may therefore play an important role in the increase of the overall drag, as further discussed below. Lower fluctuation intensities are found on the front part of the particles, where the energy dissipation is highest, and the immediate wake in the recirculating region where the instability is found to develop.

Figure 12. Contour plot of the velocity component in the direction of gravity for the single sphere settling in a quiescent fluid.
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3.4. Drag analysis

As in Maxey & Riley (1983), we write the balance of the forces acting on a single sphere settling through a turbulent flow. The equation of motion for a spherical particle reads

$$\frac{4}{3} \pi a^3 \rho_p \frac{dV_p}{dt} = \frac{4}{3} \pi a^3 (\rho_p - \rho_f) g + \oint_{\partial V_p} \tau \cdot n \, dS$$

(16)

where the integral is over the surface of the sphere $\partial V_p$, $n$ is the outward normal and $\tau = -pI + 2\mu E$ is the fluid stress. As commonly done in aerodynamics, we replace the last term of equation (16) with a term depending on the relative velocity $U_{rel}$ and a drag coefficient $C_D$

$$\frac{4}{3} \pi a^3 \rho_p \frac{dV_p}{dt} = \frac{4}{3} \pi a^3 (\rho_p - \rho_f) g - \frac{1}{2} \rho_f \pi a^2 |U_{rel}| U_{rel} C_D$$

(17)
with $\pi a^2$ the reference area. Generally, the drag coefficient $C_D$ is a function of a Reynolds number and a Strouhal number which accounts for unsteady effects. In the present case, we consider it to be a function of the Reynolds number based on the relative velocity $Re_p = 2a|U_{rel}|/\nu$ (in a turbulent field it is proper to define $Re_p$ in terms of the relative velocity between particle and fluid) and of the Strouhal number defined as

$$St = \frac{\frac{dV_p}{dt}(2a)}{|U_{rel}|^2}.$$  \hspace{1cm} (18)

The drag on the particle depends on both nonlinear and unsteady effects (such as the Basset history force and the added mass contribution) through these two non-dimensional numbers.

Commonly, the unsteady contribution is neglected and $C_D$ is assumed to depend only on the Reynolds number. Since we want to investigate both nonlinear and unsteady effects, we decide to express the drag coefficient as $C_D(Re_p, St) = C_{D0}(Re_p) [1 + \psi(Re_p, St)]$, yielding

$$4 \frac{\pi a^3 \rho_p}{3} \frac{dV_p}{dt} = 4 \frac{\pi a^3 (\rho_p - \rho_f)g - \frac{1}{2} \rho_f \pi a^2 |U_{rel}| U_{rel} C_{D0}(Re_p) [1 + \psi(Re_p, St)]}{|U_{rel}|^2},$$  \hspace{1cm} (19)

where $\psi = 0 \forall Re_p$ if $St = 0$ (steady motion). We can therefore identify a quasi-steady term and the extra term which accounts for unsteady phenomena.

By ensemble averaging equation (19) over time and the number of particles, and assuming the settling process to be at statistically steady state, we can find the most important contributions to the overall drag. The steady-state average equation reads

$$0 = 4 \frac{\pi a^3 (\rho_p - \rho_f)g - \frac{1}{2} \rho_f \pi a^2 |U_{rel}| U_{rel} C_{D0}(Re_p) [1 + \psi(Re_p, St)]}{|U_{rel}|^2} + \Psi(t).$$  \hspace{1cm} (20)

Denoting the entire time dependent term simply as $\Psi(t)$ and rearranging, we obtain the following balance

$$4 \frac{\pi a^3 (\rho_p/\rho_f - 1)g - \frac{1}{2} \rho_f \pi a^2 |U_{rel}| U_{rel} C_{D0}(Re_p)}{\rho_f} + \Psi(t).$$  \hspace{1cm} (21)

The term on the left-hand side is known whereas the time-dependent term $\Psi(t)$ is of difficult evaluation. The nonlinear steady term can be calculated using the approach described in section 3.2. At each time step we calculate the relative velocity in the spherical shells surrounding each particle. From these we compute the particle Reynolds number $Re_p = 2a|U_{rel}|/\nu$ and using equation (8) (where we replace the terminal Reynolds number with the new particle Reynolds number) we obtain the drag coefficient. The first term on the right-hand side can therefore be evaluated by averaging over the number of particles and time steps considered. Finally we divide everything by the buoyancy acceleration to estimate the relative importance of each term

$$100\% = S(Re_p) + \Psi(t).$$  \hspace{1cm} (22)
where $S(Re_p)$ represents the nonlinear steady term while the unsteady term has been denoted again as $\Psi(t)$ for simplicity.

This approach is applied to the results of the simulations of a single sphere and to the quiescent and turbulent cases with $\phi = 0.5\%$ and $1\%$. The inner radius of the sampling shells is chosen to be 5 particle radii and the results obtained are reported in table 7. The single sphere simulation provides an estimate of the error of the method. Since our terminal Reynolds number is smaller than the critical Reynolds number above which unsteady effects become important and our velocity field is indeed steady, the term $\Psi(t)$ should be negligible. The critical Reynolds number $Re_c$ has been found to be approximately 274 by Bouchet et al. (2006) while we recall that our terminal Reynolds number for the isolated particle is 200. The nonlinear steady term provides in this case, however, an overestimated value of the drag, with a percentage error of about $+3\%$ with respect to the buoyancy term. The possible causes of this error are the long wake and the fact that equation (8) is empirical. The data from the single-particle simulations are used to correct the results from the other runs, i.e. the data are normalized with the total drag obtained in this case. In the quiescent case at $\phi = 0.5\%$, unsteady effects are negligible (about $0.5\%$ of the total drag), while they increase to about $6\%$ when increasing the particle evolve fraction to $1\%$. In a turbulent flow, importantly, we notice that the contribution of $\Psi(t)$ adds up to approximately $10\%$ of the total at $\phi = 0.5\%$ and to about $12\%$ of the total at $\phi = 1\%$.

Note that one can write the steady drag as mean and fluctuating component

$$S(Re_p) = \langle |U_{rel}|U_{rel}C_{D_0}(Re_p) \rangle = \langle U_{rel} \rangle^2 C_{D_0}(\langle Re_p \rangle) + S'(\langle Re_p \rangle).$$

The fluctuations $S'(\langle Re_p \rangle)$ would be responsible of the reduction of the settling velocity if this were to be attributed to nonlinear drag effects only (see also Wang & Maxey 1993). We verified that for our results, the total and mean component differ by about $2\%$, $\langle |U_{rel}|U_{rel}C_{D_0}(Re_p) \rangle \approx \langle U_{rel} \rangle^2 C_{D_0}(\langle Re_p \rangle)$. This leads us to the conclusion that the main contribution to the overall drag is due to the steady term but the reduction of the mean settling velocity in a turbulent environment is almost entirely due to the various unsteady effects. These can be related to unsteady vortex shedding, see figure 13, as in the experiments of a single sphere by Mordant & Pinton (2000) These observations are also in agreements with the results in Homann et al. (2013). These authors observe that the enhancement of the drag of a sphere towed in a turbulent environment can be explained by the modification of the mean velocity and pressure profile, and thus of the boundary layer around the sphere, by the turbulent fluctuations.

4. Final remarks

We report numerical simulations of a suspension of rigid spherical slightly-heavy particles in a quiescent and turbulent environment using a direct-forcing immersed boundary method to capture the fluid-structure interactions. Two
dilute volume fractions, $\phi = 0.5\%$ and $1\%$, are investigated in quiescent fluid and homogeneous isotropic turbulence at $Re_\lambda = 90$. The particle diameter is of the order of the Taylor length scale and about 12 times the dissipative Kolmogorov scale. The ratio between the sedimentation velocity and the turbulent fluctuations is about 3.4, so that the strongest fluid-particle interactions occur at approximately the Taylor scale.

The choice of the parameters is inspired by the reduction in sedimentation velocity observed experimentally in a turbulent flow by Byron (2015) and in the group of Prof. Variano at UC Berkeley. In the experiment, the isotropic homogeneous turbulence is generated in a tank of dimensions of several integral lengthscales by means of two facing randomly-actuated synthetic jet arrays (driven stochastically). The Taylor microscale Reynolds number of the experiment is $Re_\lambda = 260$. Particle Image Velocimetry using Refractive-Index-Matched Hydrogel particles is used to measure the fluid velocity and the linear and angular velocities of finite-size particles of diameter of about 1.4 Taylor microscales and density ratios $\rho_p/\rho_f = 1.02, 1.006$ and $1.003$. The ratio between the terminal quiescent settling velocity $v_t$ and the turbulence fluctuating velocity $u'$ is about 1, higher than in our simulations where this ratio is 3.3. Byron (2015) observes reductions of the slip velocity between 40% and 60% when varying the shape and density of the particles. As suggested by Byron (2015), the larger reduction in settling velocity observed in the experiments is most likely explained by the larger turbulence intensity.

The new findings reported here can be summarized as follows: i) the reduction of settling velocity in a quiescent flow due to the hindering effect is reduced at finite inertia by pair-interactions, e.g. drafting-kissing-tumbling. ii) Owing to these particle-particle interactions, sedimentation in quiescent environment presents therefore significant intermittency. iii) The particle settling velocity is further reduced in a turbulent environment due to unsteady drag effects. iv) Vortex shedding and wake disruption is served also in subcritical conditions in an already turbulent flow.

In a quiescent environment, the mean settling velocity slightly decreases from the reference value pertaining few isolated particle when the volume fraction $\phi = 0.5\%$ and $\phi = 1\%$. This limited reduction of the settling velocity
Sedimentation of finite-size spheres

with the volume fraction is in agreement with previous experimental findings in inertia-less and inertial flows. The Archimedes number of our particle is 21000, in the steady vertical regime before the occurrence of a first bifurcation to an asymmetric wake. In this regime, Uhlmann & Doychev (2014) observe no significant particle clustering, which is is confirmed by the present data.

The skewness and flatness of the particle velocity reveal large positive values in a quiescent fluid, and accordingly the velocity probability distribution functions display evident positive tails. This indicates a highly intermittent behavior. In particular, it is most likely to see particles sedimenting at velocity significantly higher than the mean: this is caused by the close interactions between particle pairs (more seldom triplets). Particles approaching each other draft-kiss-tumble while falling faster than the average.

In a turbulent flow, the mean sedimentation velocity further reduces, to 0.88 and 0.86 at $\phi = 0.5\%$ and $\phi = 1\%$. The variance of both the linear and angular velocity increases in a turbulent environment and the single-particle time correlations decay faster due to the turbulence mixing. The velocity probability distribution function are almost symmetric and tend towards a Gaussian of corresponding variance. The particle lateral dispersion is, as expected, higher in a turbulent flow, whereas the vertical one is, surprisingly, of comparable magnitude in the two regimes; this can be explained by the highly intermittent behavior observed in the quiescent fluid.

We compute the averaged relative velocity in the particle reference frame and the fluctuations around the mean. We show that the wake behind each particle is on average significantly reduced in the turbulent flow and large-amplitude unsteady motions appear on the side of the sphere in the regions of minimum pressure where vortex shedding is typically observed. The effect of a turbulent flow on the damping of the wake behind a rigid sphere has been discussed for example by Bagchi & Balachandar (2003), while the case of a spherical bubble has been investigated by Merle et al. (2005). Using the slip velocity between the particle and the fluid surrounding it, we estimate the nonlinear drag on each particle from empirical formulas and quantify the relevance of non-stationary effects on the particle sedimentation. We show that these become relevant in the turbulent regime, amount to about 10-12% of the total drag, and are responsible for the reduction of settling velocity with the respect to the quiescent flow. This can be compared with the simulations in Good et al. (2014) who attribute the reduction of the sedimentation velocity of small ($2a < \eta$) heavy ($\rho_p/\rho_f \approx 900$) spherical particles in turbulence to the nonlinear drag. Here, we show that non-stationary effects become relevant for larger particles at lower density ratios.

The present investigation can be extended in a number of interesting directions. Preliminary simulations reveal that variations of the density ratio at constant Archimedes number do not significantly modify the results presented here. It would be therefore interesting to investigate the effect of the
Galilean number on the particle dynamics and of the ratio between turbulent fluctuations and sedimentation velocity.

This work was supported by the European Research Council Grant No. ERC-2013-CoG-616186, TRITOS. The authors acknowledge Prof. Variano for fruitful discussions and comments on the manuscript, computer time provided by SNIC (Swedish National Infrastructure for Computing) and the support from the COST Action MP1305: Flowing matter.
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Paper 2
The effect of particle density in turbulent channel flow laden with finite size particles in semi-dilute conditions

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Submitted to \textit{Phys. Fluids}

We study the effect of varying the mass and volume fraction of a suspension of rigid spheres dispersed in a turbulent channel flow. We performed several Direct Numerical Simulations using an Immersed Boundary Method for finite-size particles changing the solid to fluid density ratio $R$, the mass fraction $\chi$ and the volume fraction $\phi$. We find that varying the density ratio $R$ between 1 and 10 at constant volume fraction does not alter the flow statistics as much as when varying the volume fraction $\phi$ at constant $R$ and at constant mass fraction. Interestingly, the increase in overall drag found when varying the volume fraction is considerably higher than that obtained for increasing density ratios at same volume fraction. The main effect at density ratios $R$ of the order of 10 is a strong shear-induced migration towards the centerline of the channel. When the density ratio $R$ is further increased up to 100 the particle dynamics decouple from that of the fluid. The solid phase behaves as a dense gas and the fluid and solid phase statistics drastically change. In this regime, the collision rate is high and dominated by the normal relative velocity among particles.

1. Introduction

The transport of particles in flows is relevant to many industrial applications and environmental processes. Examples include sediment transport in rivers, avalanches and pyroclastic flows, as well as many oil industry and pharmaceutical processes. Often the flow regime encountered in such applications is turbulent due to the high flow rates and it can be substantially affected by the presence of the solid phase. Depending on the features of both fluid and solid phases, many different scenarios can be observed and the understanding of such flows is still incomplete.

The rheological properties of these suspensions have mainly been studied in
the viscous Stokesian regime and in the low speed laminar regime. Even limiting our attention to monodisperse rigid neutrally buoyant spheres suspended in Newtonian liquids, we find interesting rheological behaviors such as shear thinning or thickening, jamming at high volume fractions, and the generation of high effective viscosities and normal stress differences (Stickel & Powell 2005; Morris 2009; Wagner & Brady 2009). It is known that the effective viscosity of a suspension \( \mu_e \) changes with respect to that of the pure fluid \( \mu \) due to the modification of the response of the complex fluid to the local deformation rate (Guazzelli & Morris 2011). In the dilute regime, an expression for the effective viscosity \( \mu_e \) with the solid volume fraction \( \phi \) has first been proposed by Einstein (1906, 1911) and then corrected by Batchelor (1970) and Batchelor and Batchelor & Green (1972). As the volume fraction increases, the mutual interactions among particles become more important and the effective viscosity increases until the system jams (Sierou & Brady 2002). At high volume fractions, the variation of the effective viscosity \( \mu_e \) is described exclusively by semi-empirical laws such as those by Eiler and Krigher & Dougherty (Stickel & Powell 2005) that also capture the observed divergence at the maximum packing limit, \( \phi_m = 0.58 - 0.62 \) (Boyer et al. 2011). In laminar flows, shear-thickening or normal stress differences occur due to inertial effects at the particle scale. Indeed, when the particle Reynolds number \( Re_a \) is non negligible the symmetry of the particle pair trajectories is broken and the microstructure becomes anisotropic, leading to macroscopical behaviors such as shear-thickening (Kulkarni & Morris 2008; Picano et al. 2013; Morris & Haddadi 2014). In the highly inertial regime the effective viscosity \( \mu_e \) increases linearly with shear rate due to augmented particle collisions (Bagnold 1954).

Another important feature observed in viscous flows is shear-induced migration. When considering a pressure-driven Poiseuille flow, either in a tube or in a channel, the particles irreversibly migrate toward the centerline, i.e. from high to low shear rate regions (Guazzelli & Morris 2011; Koh et al. 1994). Interestingly when inertial effects become important, a different kind of migration occurs as the particles tend to move radially away from both the centerline and the walls, toward an intermediate equilibrium position. This type of migration was first observed in a tube (Guazzelli & Morris 2011; Segre & Silberberg 1962) and was named tubular pinch. It is mechanistically unrelated to the rheological properties of the flow and results from the fluid-particle interaction within the conduit. The case of the laminar square duct flow has also been studied to identify the particle equilibrium position (Chun & Ladd 2006; Abbas et al. 2014).

Further increasing the Reynolds number, inertial effects become more important until the flow undergoes a transition from laminar to turbulent conditions. The presence of the solid phase may alter this process, for example, by either increasing or reducing the critical Reynolds number above which the transition to the turbulent regime occurs. The case of a dense suspension of particles in a pipe flow has been studied experimentally (Matas et al. 2003)
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and numerically (Yu et al. 2013). It has been suggested that transition depends upon the pipe to particle diameter ratios and the volume fraction. Transition shows a non-monotonic behavior and may be either anticipated or delayed, a behavior that cannot be explained in terms of an increase of the effective viscosity. The transition in dilute suspensions of finite-size particles in plane channels has been studied by Lashgari et al. (2015a) and Loisel et al. (2013). It has been shown that the critical Reynolds number above which turbulence is sustained, is reduced. At fixed Reynolds number and solid volume fraction, the initial arrangement of particles is important to trigger the transition. Channel flow at higher volume fractions has been numerically investigated in Lashgari et al. (2014), where three different regimes are identified for different values of the solid volume fraction $\phi$ and the Reynolds number $Re$. In each regime (laminar, turbulent and inertial shear-thickening), the flow is dominated by different components of the total stress (viscous, turbulent or particle stresses respectively).

Most of the previous studies in the fully turbulent regime have focused on dilute or very dilute suspensions of particles smaller than the hydrodynamic scales and heavier than the fluid. In the one-way coupling regime (Balachandar & Eaton 2010) (i.e. when the solid phase has a negligible effect on the fluid phase) and limiting our attention to wall-bounded flows, it has been shown that particles migrate from regions of high to low turbulence intensities (Reeks 1983). This phenomenon is known as turbophoresis and it has been shown to be stronger when the turbulent near-wall characteristic time and the particle inertial time scale are similar (Soldati & Marchioli 2009). Small-scale clustering has also been observed in this kind of inhomogeneous flows (Sardina et al. 2012), leading together with turbophoresis to the formation of streaky particle patterns (Sardina et al. 2011). In the two-way coupling regime (i.e. when the mass density ratios are high and the back-reaction of the dispersed phase on the fluid cannot be neglected) the solid phase has been shown to reduce the turbulent near-wall fluctuations increasing their anisotropy (Kulick et al. 1994) and eventually reducing the total drag (Zhao et al. 2010).

When the suspensions are dense it is of fundamental importance to consider particle-particle interactions and collisions. The chaotic dynamics of the fluid phase affects the rheological properties of the suspension, especially at high Reynolds numbers. This is known as a four-way coupling regime. Increasing the particle size directly affects the turbulent structures at smaller and comparable scales (Naso & Prosperetti 2010) thereby modulating the turbulent field. In a turbulent channel flow it has been reported that finite-size particles larger than the dissipative length scale increase the turbulent intensities and the Reynolds stresses (Pan & Banerjee 1996). Particles are also found to preferentially accumulate in the near-wall low-speed streaks (Pan & Banerjee 1996). This has also been observed in open channel flows laden with heavy finite-size particles. In this case the flow structures are found to have a smaller streamwise velocity (Kidanemariam et al. 2013; Kidanemariam & Uhlmann 2014).
Concerning turbulent channel flows of neutrally buoyant particles with \( \phi \simeq 7\% \), recent studies report that due to the attenuation of the large-scale streamwise vortices, the fluid streamwise velocity fluctuation is reduced. When the particles are heavier than the carrier fluid and therefore sediment, the bottom wall acts as a rough boundary which makes the particles resuspend (Shao et al. 2012). Recent simulations from our group have shown that the overall drag increases as the volume fraction is increased from \( \phi = 0\% \) up to 20\%. This trend cannot be solely explained in terms of the increase of the suspension effective viscosity. It is instead found that as particle volume fraction increases, the velocity fluctuation intensities and the Reynolds shear stresses decrease while there is a significant increase of the particle induced stresses. The latter, in turn, lead to a higher overall drag (Picano et al. 2015).

As noted by Prosperetti (2015), results obtained for solid to fluid density ratios \( R = \rho_p / \rho_f = 1 \) cannot be easily extrapolated to other cases (e.g. when \( R > 1 \)). In the present study we therefore investigate numerically the effects of varying the density ratio \( R \) of the suspended phase and consequently the mass fraction \( \chi \) for different volume fractions. The main aim is to understand separately the effects of excluded volume and (particle and fluid) inertia on the statistical observables of both phases. To isolate the effects of different density ratios \( R \) on the macroscopical behavior of the suspension, we consider an ideal situation where the effect of gravity is neglected, leaving its analysis to future studies.

We consider a turbulent channel flow laden with rigid spheres of radius \( a = h/18 \) where \( h \) is the half-channel height (see Picano et al. (2015)). Direct numerical simulations (DNS) fully describing the solid phase dynamics via an immersed boundary method (IBM) are performed as in Lucci et al. (2010) and Kidanemariam et al. (2013) among others. First, cases at fixed mass fractions \( \chi = 0.2 \) are examined and compared to cases with constant volume fraction \( \phi = 5\% \) and density ratios \( R \) ranging from 1 to 10. It is observed that the influence of the density ratio \( R \) on the statistics of both phases is less important than that of an increasing volume fraction \( \phi \). The main effects at density ratio \( R \sim 10 \) are shear-induced migration towards the centerline of the channel and slight reduction of the fluid velocity fluctuations in the log-layer. The results drastically change when further increasing \( R \) (up to \( \sim 100 \)) no matter the volume fraction. With a second set of simulations performed at constant \( \phi = 5\% \) but varying \( R \), it is found that for sufficiently high \( R (\sim 100) \), the fluid and solid phases decouple. The solid phase behaves as a dense gas uncorrelated to the details of the carrier fluid flow.

2. Methodology

2.1. Numerical method

Different methods have been proposed in the last years to perform Direct Numerical Simulations of multiphase flows. In the present study, simulations have been performed using the algorithm originally developed by Breugem (2012).
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that fully describes the coupling between the solid and fluid phases. The Eulerian fluid phase is evolved according to the incompressible Navier-Stokes equations,

$$\nabla \cdot \mathbf{u}_f = 0$$  

(1)

$$\frac{\partial \mathbf{u}_f}{\partial t} + \mathbf{u}_f \cdot \nabla \mathbf{u}_f = -\frac{1}{\rho_f} \nabla p + \nu \nabla^2 \mathbf{u}_f + \mathbf{f}$$  

(2)

where $\mathbf{u}_f$, $\rho_f$ and $\nu = \mu/\rho_f$ are the fluid velocity, density and kinematic viscosity respectively ($\mu$ is the dynamic viscosity), while $p$ and $\mathbf{f}$ are the pressure and a generic force field (used to model the presence of particles). The particles centroid linear and angular velocities, $\mathbf{u}_p$ and $\omega_p$ are instead governed by the Newton-Euler Lagrangian equations,

$$\rho_p V_p \frac{d\mathbf{u}_p}{dt} = \rho_f \oint_{\partial V_p} \tau \cdot \mathbf{n} \, dS$$  

(3)

$$I_p \frac{d\omega_p}{dt} = \rho_f \oint_{\partial V_p} \mathbf{r} \times \tau \cdot \mathbf{n} \, dS$$  

(4)

where $V_p = 4\pi a^3/3$ and $I_p = 2\rho_p V_p a^2/5$ are the particle volume and moment of inertia; $\tau = -p\mathbf{I} + 2\mu\mathbf{E}$ is the fluid stress, with $\mathbf{E} = (\nabla \mathbf{u}_f + \nabla \mathbf{u}_f^T)/2$ the deformation tensor; $\mathbf{r}$ is the distance vector from the center of the sphere while $\mathbf{n}$ is the unity vector normal to the particle surface $\partial V_p$. Dirichlet boundary conditions for the fluid phase are enforced on the particle surfaces as $\mathbf{u}_f|_{\partial V_p} = \mathbf{u}_p + \omega_p \times \mathbf{r}$.

In the numerical code, an immersed boundary method is used to couple the fluid and solid phases. The boundary condition at the moving particle surface (i.e. $\mathbf{u}_f|_{\partial V_p} = \mathbf{u}_p + \omega_p \times \mathbf{r}$) is modeled by adding a force field on the right-hand side of the Navier-Stokes equations. The fluid phase is therefore evolved in the whole computational domain using a second order finite difference scheme on a staggered mesh while the time integration is performed by a third order Runge-Kutta scheme combined with a pressure-correction method at each sub-step. The same integration scheme is also used for the Lagrangian evolution of eqs. (4) and (5). Each particle surface is described by uniformly distributed $N_L$ Lagrangian points. The force exchanged by the fluid on the particles is imposed on each $l-th$ Lagrangian point and is related to the Eulerian force field $\mathbf{f}$ by the expression $\mathbf{f}(\mathbf{x}) = \sum_{l=1}^{N_L} \mathbf{F}_l \delta_d(\mathbf{x} - \mathbf{X}_l) \Delta V_l$. In the latter $\Delta V_l$ represents the volume of the cell containing the $l-th$ Lagrangian point while $\delta_d$ is the Dirac delta. This force field is calculated through an iterative algorithm that ensures a second order global accuracy in space. In order to maintain accuracy, eqs. (4)
and (5) are rearranged in terms of the IBM force field,

$$\rho_p V_p \frac{d\mathbf{u}_p}{dt} = -\rho_f \sum_{l=1}^{N_l} \mathbf{F}_l \Delta V_l + \rho_f \frac{d}{dt} \int_{V_p} \mathbf{u}_f \, dV$$  \hspace{1cm} (5)$$

$$I_p \frac{d\omega_p}{dt} = -\rho_f \sum_{l=1}^{N_l} \mathbf{r}_l \times \mathbf{F}_l \Delta V_l + \rho_f \frac{d}{dt} \int_{V_p} \mathbf{r} \times \mathbf{u}_f \, dV$$  \hspace{1cm} (6)$$

where $r_l$ is the distance from the center of a particle while the second terms on the right-hand sides are corrections to account for the inertia of the fictitious fluid contained within the particle volume. Particle-particle interactions are also considered. When the gap distance between two particles is smaller than twice the mesh size, lubrication models based on Brenner’s asymptotic solution (Brenner 1961) are used to correctly reproduce the interaction between the particles. A soft-sphere collision model is used to account for collisions between particles and between particles and walls. An almost elastic rebound is ensured with a restitution coefficient set at 0.97. These lubrication and collision forces are added to the right-hand side of eq. (6). For more details and validations of the numerical code, the reader is referred to previous publications (Breugem 2012; Lambert et al. 2013; Picano et al. 2015; Fornari et al. 2015).

### 2.2. Flow configuration

We consider a turbulent channel flow between two infinite flat walls located at $y = 0$ and $y = 2h$, where $y$ is the wall-normal direction while $x$ and $z$ are the streamwise and spanwise directions. The domain has size $L_x = 6h$, $L_y = 2h$ and $L_z = 3h$ and periodic boundary conditions are imposed in the streamwise and spanwise directions. A fixed value of the bulk velocity $U_0$ is achieved by imposing a mean pressure gradient in the streamwise direction. The imposed bulk Reynolds number is equal to $Re_b = U_0 2h/\nu = 5600$ (where $\nu$ represents the kinematic viscosity of the fluid) and corresponds to a Reynolds number based on the friction velocity $Re_\tau = U_* h/\nu = 180$ for the single phase case. The friction velocity is defined as $U_* = \sqrt{\tau_w/\rho_f}$, where $\tau_w$ is the stress at the wall. A cubic staggered mesh of $864 \times 288 \times 432$ grid points is used to discretize the domain. All results will be reported either in non-dimensional outer units (scaled by $U_0$ and $h$) or in inner units (with the superscript ‘+’, scaled by $U_*$ and $\delta_* = \nu/U_*$).

The solid phase consists of non-Brownian neutrally buoyant rigid spheres with a radius to channel half-width ratio fixed to $a/h = 1/18$. For a volume fraction $\phi = 5\%$, this radius corresponds to about 10 plus units. In figure 1 we display the instantaneous streamwise velocity on four orthogonal planes together with the finite-size particles dispersed in the domain. Each particle is discretized with $N_l = 746$ Lagrangian control points while their radii are 8 Eulerian grid points long.

At first, we will compare results obtained at different density ratios $R$ and constant mass fraction $\chi$ with those at constant volume fraction $\phi$. The mass
fraction is defined as $\chi = \phi R$ and is chosen to be 0.2: four simulations are performed with $R = 1, 4, 10, 100$ and $\phi = 20\%, 5\%, 2\%, 0.2\%$ (which correspond to 10000, 2500, 1000 and 100 particles). At constant $\phi = 5\%$ instead, we examine four cases with $R = 1, 2, 4$ and 10. The reference unladen case ($\phi = 0\%$) is also presented in the different figures. The case with $\phi = 5\%$ and $R = 100$ will be discussed later. The full set of simulations is summarized in table 1.

The simulations start from the laminar Poiseuille flow for the fluid phase. Transition to turbulence naturally occurs at the fixed Reynolds number due to the noise added by the presence of the solid phase. Particles are initially positioned randomly with velocity equal to the local fluid velocity. Statistics are collected after the initial transient phase.

3. Results

3.1. Analysis of Mass and Volume Fraction Effects

We show the mean fluid velocity profiles in outer and inner units ($U^+_f = U_f / U_*$ and $y^+ = y/\delta_*$) in figure 2. The statistics conditioned to the fluid phase have been calculated neglecting the points occupied by the solid phase in each field (phase-ensemble average). We notice in 2(a) and (c) that the velocity profile tends towards that for the single fluid phase as the volume fraction is reduced even if the mass fraction $\chi$ is constant. Conversely, when the volume fraction is kept constant at 5% (panels b and d) the differences observed when increasing the density ratios are small; in particular smaller velocities near the wall and larger velocities in the centre of the channel for larger $\chi$. The decrease of the profiles in inner units, observed when increasing $\phi$ and less so increasing $R$ at fixed $\phi$, indicates also an overall drag increase. Indeed for $y^+ > 40 – 50$ the mean profile follows the log-law (Pope 2000):

$$U^+ = \frac{1}{k} \log (y^+) + B$$ (7)
where $k$ and $B$ are the von Kármán constant and an additive coefficient. As $R$ increases, $k$ is found to decrease from 0.36 to 0.29 while $B$ is reduced from 2.7 to $-1.3$ (see figure 2d). Usually a decrease in $k$ denotes drag reduction while a smaller or negative $B$ leads to an increase in drag (Virk 1975). In the cases studied this combined effect leads to a small increase of the overall drag since the friction Reynolds number $Re_\tau$ grows from 195 to 203. The reduction in the additive coefficient $B$ is believed to be caused by the intense particle-fluid interactions occurring near the wall (Picano et al. 2015), which are augmented by the increased inertia of the solid phase at higher $R$.

We report in table 2 the values of $k, B$ and $Re_\tau$ obtained for all the cases studied. For the case with $\phi = 0.2\%$ and $R = 100$ (yet $\chi = 0.2$) we almost recover the single phase log-law with $k = 0.38$ and $B = 4.7$ (for the single fluid $k = 0.4$ and $B = 5.5$) and the increase in friction Reynolds number $Re_\tau$ is limited (from 180 to 183), which can be explained by the small number of particles in the flow. As shown above, the cases at the same mass fraction ($\chi = 0.2$) and different density ratios reveal most significant variations, explained by the changes in volume fraction $\phi$ (excluded volume effect).

The root-mean-square (r.m.s.) of the fluid velocity fluctuations are reported in inner units in figure 3. Panels (a),(c) and (e) show the cases at constant $\chi$ while the cases at constant $\phi$ are reported in panels (b),(d) and (f). As for the mean flow, the major changes in fluid velocity fluctuations are associated to an increase in volume fraction $\phi$. As $\phi$ is increased from $0.2\%$ to $5\%$ (constant $\chi$), the wall-normal $v'_{f,rms}$ and spanwise components $w'_{f,rms}$
The effect of particle density

**Figure 2.** Mean fluid streamwise velocity profiles for constant \( \chi = 0.2; \) (a) data scaled in outer units and (c) inner units. The corresponding cases at constant \( \phi = 0.05 \) are displayed in (b) and (d).

increase especially in the proximity of the wall, i.e. in the viscous sublayer. We observe also an important reduction of the streamwise fluctuation intensity around \( y^+ = 10 \) at higher \( \phi \). As we will show later, a layer of particles is formed close to the walls and the fluid between these particles and the walls is therefore squeezed. This results in a reduction of the streamwise fluid velocity fluctuations and an increase of the fluctuations in the other directions. The neutrally buoyant case at higher volume fractions (\( \phi = 20\% \), \( R = 1 \)) exhibits higher fluctuations close to the walls that drop well below the values found for the smaller volume fractions \( \phi \) as \( y^+ \) is further increased. Only the streamwise component \( u_{f,rms}^{+} \) approaches the values obtained at smaller \( \phi \) when \( y^+ > 80 \).

The fluid velocity fluctuation profiles do not show a significant dependence on the density ratio \( R \). However, one can notice that increasing the density ratio to \( R = 10 \) leads to a reduction of the fluctuation intensities in all directions (when \( y^+ > 5 \)), similarly to what observed at \( R = 1 \) and increasing \( \phi \) (see previous discussion or the work by Picano and collaborators (Picano et al. 2015) for a more complete discussion). Important differences are found for \( y^+ < 5 \) (i.e. very close to the wall) where the velocity fluctuations increase when increasing the volume fraction while they remain approximately constant when varying \( R \).
As mean velocity profiles are affected mostly by variations in the solid volume fraction $\phi$, the explanation for the change in fluid velocity fluctuations must be searched in the context of fluid-solid interactions and of the suspension microstructure. We therefore report in figure 4 the local solid volume fraction along the wall-normal direction $\phi(y)$. It is evident that for $R > 1$ a layer of particles forms close to the walls as soon as the volume fraction $\phi$ is above 0.2%.

As shown in figure 4(b) for a constant volume fraction ($\phi = 5\%$), as the density ratio increases more particles tend to migrate toward the centerline while the layer close to the wall is preserved. The peak of $\phi(y)$ close to the wall is slightly reduced and less particles occupy the volume between $y \sim 0.1$ and 0.6. We therefore observe a shear-induced particle migration from regions of high to low shear rates, an effect more pronounced as the density ratio $R$ increases. The local volume fraction increases drastically at the centerline ($y = 1$): the local volume fraction at the centerline $\phi(y = 1)$ is approximately twice that found at $y \sim 0.1$ (i.e. close to the wall where the first layer of particles form) when $R = 4$. The difference is even higher when $R = 10$– $\phi(y = 1) \simeq 5\phi(y = 0.1)$. This shear-induced migration becomes more intense as the density ratio $R$ increases although, as we will see later, the picture totally changes at very high $R$ ($\sim 100$).

We report the mean particle streamwise velocity $U_p$ in figure 5. The results for constant $\chi$ are shown in panel (a) where we notice that the mean particle streamwise velocity profiles are similar for $\phi = 2\%$ and 5% when $R = 10$ and 4. For $\phi = 0.2\%$ and $R = 100$ instead, the mean particle streamwise velocity profile changes drastically showing higher velocities close to the wall and smaller velocities in the rest of the channel ($y \geq 0.3$). Comparing with the other cases we find a 13% reduction of $U_p$ at the centerline. Generally we find that as the

<table>
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<th>$\chi$</th>
<th>$\phi(%)$</th>
<th>$R$</th>
<th>$k$</th>
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Table 2. Summary of the values of the von Kármán constant $k$, the additive coefficient $B$ and the friction Reynolds number $Re_\tau$ obtained for the cases studied. The reference case with no dispersed phase is also reported. Here $k$ and $B$ have been fitted in the range $y^+ \in [50, 150]$.  

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Figure 3. Intensity of the fluctuation velocity components for the fluid phase in inner units. (a),(c),(e) simulations at constant mass fraction $\chi = 0.2$. (b),(d),(f) Data at constant volume fraction $\phi = 0.05$.

When the volume fraction $\phi$ is fixed (fig. 5b), $U_p$ is only slightly altered by an increase in density ratio $R$. However, at the highest density ratio ($R = 10$) particles move faster in proximity of the walls and around the centerline while $U_p$ is reduced between these two regions. The particles that lie in this region have a streamwise velocity directly linked to that of the fluid, while particles are
accelerated in proximity of the wall and around the centerline where collision are more frequent.

In figure 6 we show the instantaneous particle positions from the simulation with $R = 10$ projected in the streamwise-wall-normal ($x - y$) plane. The interaction between two approaching particles slightly shifted in the wall-normal direction and in the proximity of the wall is also sketched to explain shear-induced inertial migration. In this high shear rate region, the particle denoted by $a$, with velocity $U_{p,a}$, approaches particle $b$, moving in the same direction with velocity $U_{p,b}$. Since the latter is closer to the wall, its streamwise velocity $U_{p,b}$ is smaller (on average) than that of particle $a$, so a collision takes place. The scenario following this collision depends on the inertia of the fluid and solid phases, and thereby on the density ratio $R$.

If particles $a$ and $b$ are neutrally buoyant $R = 1$, their dynamics is mainly determined by the carrier fluid flow. After the collision, the two particles would tend to move radially apart and their motion becomes rapidly correlated to that of the fluid phase. As a result, they are on average transported downstream by the flow. As the particle inertia increases (i.e. $R$ increases), the particle motion
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Figure 6. Instantaneous particle positions in the $x-y$ plane from the simulation with $R = 10$. On top, a sketch explaining the observed shear-induced migration is also presented.

is less sensitive to the fluid flow and longer times are needed for the particle to adjust to the fluid velocity after the collision. Indeed, for $R \geq 4$, the particle relaxation time is longer than the fluid timescale. Therefore, particles migrate almost undisturbed in opposite wall-normal directions after a collision. Owing to the presence of the wall, we therefore observe a net migration towards the channel centre. Being this an inertial effect, the particle migration is more evident as the solid to fluid density ratio $R$ increases. As we will discuss later, however, this effect disappears at very high density rations, $R$, when the particle mean velocity is almost uniform, and there is no a mean shear. On average, this inertial shear-induced migration leads to high peaks of the local solid volume fraction $\phi(y)$ at the centerline (see figure 4 b). The effect is so strong at $R = 10$, that it is easy to identify intermittently depleted regions of particles close to the walls (as shown in the snapshot in figure 6).

A similar wall-normal particle migration has been observed for dense suspensions ($\phi = 30\%$) of neutrally buoyant rigid spherical particles at bulk Reynolds numbers $Re_b$ ranging from 500 to 5000 (Lashgari et al. 2015b). In these cases, the profiles of local volume fraction, $\phi(y)$, do not vary significantly by increasing the bulk Reynolds number and the observed migration has been attributed to the imbalance of normal stresses in the wall-normal direction. Although the resulting behavior is similar, the driving mechanisms are different.

In this section we have studied the dependence of the suspension properties on both the solid to fluid density ratio $R$ and the solid volume fraction $\phi$. We have shown that the mean and fluctuating velocity fields of both phases are predominantly influenced by variations in the volume fraction $\phi$ (i.e. excluded volume effects). The mean fields are only marginally altered by increasing the
3.2. Effects of Density Ratio $R$

In this section we discuss the results obtained in an idealized scenario where the density ratio is allowed to further increase while gravity effects are neglected. We compare results obtained at $\phi = 5\%$ and $R = 1, 10$ and $100$ showing that above a certain density ratio ($R > 10$), the solid phase decouples from the fluid leading to a completely different scenario.

3.2.1. Single-point statistics

The streamwise fluid velocity profiles in outer and inner units (panels (a) and (b)), the particle streamwise velocity profile (panel (c)) and the local volume fraction profile $\phi(y)$ (panel (d)) are displayed in figure 7 for $\phi = 5\%$ and increasing particle density.

The mean fluid and particle velocity $U_p$ changes significantly at the highest density ratio considered, $R = 100$. The fluid velocity increases more rapidly
from the wall and reaches a constant value slight above 1 for $y \gtrsim 0.3$. This value is about 12% smaller than what found at the centerline for the cases with lower density ratio. The difference between the different profiles is even more evident when the data are scaled with inner units (fig. 7b). As already mentioned in the previous section, the mean velocity profiles are similar for density ratios between 1 and 10, still giving different coefficients for the fitting of the log-law. The velocity profiles almost overlap in the viscous sublayer and converge to approximately the same values of $U_f^+$ for $y^+ > 100$. For the case
with $R = 100$, instead, the mean velocity is close to that for $R = 10$ only close to the wall, $y^+ \lesssim 20$.

Larger differences are found for the solid phase velocity, figure 7(c): the average streamwise particle velocity is constant and approximately equal to 1, the bulk value. This is similar to the behavior previously reported for $\phi = 0.2\%$ and $R = 100$. All particles move in average with the same streamwise velocity, no matter if they are close to the walls or to the centerline. Their motion seems not to be affected by turbulent fluid flow. The solid and fluid phases seem indeed decoupled and a pseudo-plug flow of particles is generated across the channel, as confirmed by the local volume fraction profile, $\phi(y)$, shown in figure 7(d). Indeed, the particles are distributed almost uniformly across the channel, with the first particle layer appearing at approximately 2 particle radii from the walls.

As discussed in the previous section, particle inertia and near-wall shear induce particle migration toward the centerline when $R = 10$. This effect becomes more evident as the density of the particles increases, until for very high $R$, their inertia is so high that their motion almost completely decouples from the one of the fluid phase. In this granular-like regime particles move ballistically between successive collisions and almost uniformly downstream with also an uniform wall-normal distribution. The turbulent flow structures are disrupted by these heavy particles and the typical features of a turbulent channel flow are lost.

It is now interesting to look at the particle Stokes number $St_p$, the ratio between the particle time scale, due to the particle inertia, and a characteristic flow time scale. We consider the convective time as flow characteristic time, $\tau_f = h/U_0 = 2h^2/(Re_b\nu)$, while the particle relaxation time is $\tau_p = 4a^2R/18\nu$. The effect of finite inertia (i.e. of a non negligible Reynolds number) should be taken into account in the definition of the particle Stokes number and we therefore consider the following correction of the particle drag coefficient $C_D$ to account for inertial effects (Schiller & Naumann 1935)

$$C_D = \frac{24}{Re_p} \left(1 + 0.15 Re_p^{0.687}\right)$$

(8)

(where $Re_p$ is the particle Reynolds number) so that the modified Stokes number

$$St'_p = \frac{\tau_p}{\tau_f \left(1 + 0.15 Re_p^{0.687}\right)} = \left(\frac{2a}{h}\right)^2 \frac{1}{36} \frac{Re_b R}{1 + 0.15 Re_p^{0.687}}.$$

(9)

For sake of simplicity and in first approximation we define a shear-rate based particle Reynolds number $Re_p = Re_b(a/h)^2 \sim 20$. The modified Stokes number $St'_p$ then becomes equal to 0.9, 8.8 and 88.3 for $R = 1, 10$ and 100. As expected, particle inertia becomes more and more relevant as the density ratio increases. For $R \in [1, 10]$ the inertia of the fluid and solid phases is comparable and they mutually influence each other. When $R = 100$, conversely, the particle Stokes number is much larger than 1 and particles are only slightly affected by
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The fluid phase. The solid phase behaves as a dense gas, uncorrelated to the fluid phase.

In figure 8 we compare the fluid and particle velocity fluctuations for the three different density ratios under investigation. It can be seen from the plots in 8(a),(c) and (e) that the fluid velocity fluctuations are significantly different at the highest $R$. All velocity components display larger values close to the wall and then drop rapidly to a constant value of approximately 0.02. Anisotropy in the energy distribution is maintained very close to the walls only, whereas a quasi-isotropic energy distribution is found in the rest of the channel. The particle velocity fluctuations reported in panels (b), (d),(f) also exhibit an almost isotropic distribution, with a fluctuation intensity of about 0.04. This statistical isotropy is typical of gaseous systems and due to the strong influence of the solid phase on the fluid phase (previously explained by means of the particle Stokes number), the fluid velocity fluctuations are forced to approach a quasi-isotropic statistical steady state.

We finally observe that, approaching the centerline, particle and fluid velocity fluctuations pertaining the case with $R = 10$ are smaller than those of the neutrally buoyant case. On average, particles are more likely to be at the channel centre and move in the direction of the pressure gradient. Fluctuations, in all directions, are therefore reduced, and due to the strong coupling between the two phases, the fluid velocity fluctuations also decrease in this more ordered structure.

3.2.2. Particle Dispersion

Next, we discuss the particle dispersion in the streamwise and spanwise directions. The motion of the particles is constrained in the wall-normal direction by the presence of the walls and is therefore not examined here. The dispersion is quantified by the variance of the particle displacement as function of
the separation time $t$. Here, we compute the mean-square displacement of the particle trajectories

$$
\langle \Delta X^2_p(t) \rangle = \langle [X_p(\bar{t} + t) - X_p(\bar{t})]^2 \rangle_{p,\bar{t}}
$$

(10)

where the square displacements are averaged over time $\bar{t}$ and the number of particles $p$.

Figure 9(a) shows the particle dispersion in the streamwise direction, $\langle \Delta x^2_p \rangle$, while the spanwise dispersion, $\langle \Delta z^2_p \rangle$, is reported in panel (b) of the same figure.

Dispersion in the streamwise direction is similar for the cases with $R = 1$ and 10. The particle trajectories are initially correlated and the displacements proportional to time $t$. In this so-called ballistic regime, the mean square dispersion $\langle \Delta x^2_p \rangle$ shows a quadratic dependence on time. Only after $t \sim 100 (2a)/U_0$, the curve approaches the linear behavior typical of a diffusive motion. This is induced by particle-particle and hydrodynamic interactions that decorrelate the trajectories in time.

As discussed above, the motion of the solid phase is almost uncorrelated to that of the fluid when increasing the density ratio to $R = 100$. Since the mean particle velocity is flat across the channel, the dispersion is not enhanced by the inhomogeneity of the velocity profile typical of shear flows, the so-called Taylor-Aris dispersion (Taylor 1953; Aris 1956). Therefore $\langle \Delta x^2_p \rangle$ is approximately one or two orders of magnitude lower than in the two cases at lower $R$. Interestingly, the purely diffusive behavior is attained faster and the transition from the ballistic behavior begins already at $t \approx 20 (2a)/U_0$.

The dispersion in the spanwise direction, $\langle \Delta z^2_p \rangle$, is similar for all density ratios $R$ considered. Again, one can identify a quadratic and linear behavior in time with a transition between the two regimes at $t \sim 20 (2a)/U_0$. We also note that, for $t \lesssim 10 (2a)/U_0$ the spanwise dispersion of the particles of highest density is close to that of particles with $R = 10$, while for $t \gtrsim 200 (2a)/U_0$ the behavior appears similar to that found for $R = 1$.

To conclude this section, we emphasize that the statistics of particle dispersion reveal that the particle motion only slightly changes when increasing the particle density ratio from $R = 1$ to $R = 10$, supporting the observation that the bulk flow behavior depends more on the excluded volume, i.e. $\phi$, rather than on the particle inertia.

3.2.3. Particle velocity probability density functions and collision rates

We wish to give further insight on the behavior of the solid phase dynamics by examining the velocity probability density functions. We will focus on the case with $R = 1, 10$ and 100 and and calculate the probability density function $p(\cdot)$ for each component of the particle velocity in the volume around the centerline of the channel (of size $2h \times 2h/3 \times 3h$). The distributions of the streamwise, wall-normal and spanwise components of the particle velocity are depicted in panels (a),(b) and (c) of figure 10.
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Figure 10. Probability density function of the particle velocity around the center of the channel, for the different density ratios under investigation (panels a, b and c for the streamwise, wall-normal and spanwise components respectively). Panel (d) reports the probability density function of the magnitude of the particle velocity fluctuations around the center of the channel where a Maxwell-Boltzmann distribution is used to fit the case with $R = 100$.

We see in panel (a) that the distribution pertaining the streamwise component, $p(u)$, exhibits a negative skewness $S (=-0.77$ and $-1.54$) for $R = 1$ and 10, indicating that particles exhibit with higher probability intense fluctuations lower than the mean value, as observed also in single-phase turbulent channel flow (Kim et al. 1987). As $R$ is increased from 1 to 10, the variance $\sigma^2$ is however reduced, whereas the flatness $F$ increases (from 3.8 to 6.9) indicating that rare events become more frequent. The results for $R = 100$ show that the velocity distribution changes to what, at first sight, may seem a normal distribution with smaller modal value and variance, almost vanishing skewness ($S \sim 0.03$) and flatness close to 3 ($F \sim 3.3$).

The velocity distributions in the cross-stream directions (reported in panels b and c) resemble a normal distribution centered around a zero mean value. As for the streamwise component, the flatness $F$ exhibits high values (between
6 and 7) only for $R = 10$ while for the remaining two cases it is just slightly greater than 3.

Next, we report the probability distributions of the modulus of the velocity fluctuations,

$$|v'| = \sqrt{u'_{p,rms}^2 + v'_{p,rms}^2 + w'_{p,rms}^2},$$

(11)
calculated in the same volume around the centerline in figure 10(d). The most peculiar distribution is the one found for $R = 100$. It closely resembles a Maxwell-Boltzmann distribution (or a $\chi$ distribution with three degrees of freedom) defined as follows:

$$p(x) = \frac{2}{\pi a^3} x^2 e^{-x^2/(2a^2)},$$

(12)

where $a$ is a scale parameter (velocity). This distribution describes the velocity of atoms of an ideal gas that freely move inside a stationary container. In such case the scale parameter becomes $a = \sqrt{kT/m}$ where $k$ is the Boltzmann’s constant, $T$ the thermodynamic temperature and $m$ the particle mass. Fitting our results with equation 12 we find $a \sim 0.037$, corresponding to the Maxwell-Boltzmann distribution displayed in panel (d) with dashed line. The root mean square of such a distribution is $\sigma = \sqrt{3a} = 0.064$, using the value of $a$ previously reported. Examining again figure 8(b),(d),(f), we notice that the velocity fluctuations are approximately equal to 0.04, with modulus $|v'| \approx 0.069$. Thus the root mean square $\sigma$ is completely defined by $|v'|$. These findings further confirm our previous speculations about the appearance of a dense gaseous regime at high density ratios $R$.

Finally we examine particle-pair statistics, function of the distance between the centers $r$, and show that the large variations of the particle velocity also affect the particle-pair dynamics, in particular the collisions. As the distance $r$ approaches the particle diameter, the near field interactions become important and collisions may occur (whenever $r = 2a$). An indicator of the radial separation among pair of particles is the Radial Distribution Function RDF. In a reference frame with origin at the centre of a particle, the RDF is the average number of particle centers located in the shell of radius $r$ and thickness $\Delta r$, normalized with the number of particles of a random distribution. Formally the RDF is defined as

$$RDF(r) = \frac{1}{4\pi} \frac{dN_r}{dr} \frac{1}{r^2 n_0},$$

(13)

where $N_r$ is the number of particle pairs on a sphere of radius $r$, $n_0 = N_p(N_p - 1)/(2V)$ is the density of particle pairs in the volume $V$, with $N_p$ the total number of particles. The value of the RDF at distances of the order of the particle radius reveals the intensity of clustering; the RDF tends to 1 as $r \to \infty$, corresponding to a random (Poissonian) distribution.

Here, we are mainly interested in the particle-pair statistics around the centerline, and therefore compute the RDF in the volume defined by $y \in$
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Figure 11. (a) Radial distribution function, (b) average negative relative velocity and (c) collision kernel (see text for the definitions) around the centerline for the three values of the density ratio $R$ indicated and particle volume fraction $\phi = 5\%$. Distances are normalized by the particle radius.

[0.67, 1.33] for the three density ratios $R = 1, 10$ and 100 and volume fraction $\phi = 5\%$. The data obtained are shown in figure 11(a). At lower density ratios, $R = 1$ and 10, the peaks of the RDF’s are found at exactly 2 particle radii from the centre of the reference particles. The RDF drops quickly to the value of the uniform distribution (i.e. 1) at $r \sim 2.25a$ in the neutrally buoyant case, whereas the decay is somewhat slower for $R = 10$, reaching the final plateau at $r \sim 3$. This difference can be explained by the shear-induced migration previously discussed: this enhances the number of particles around the centerline, thus increasing the local volume fraction and consequently the small scale clustering. At the highest density ratio under investigation, instead, the gaseous behavior of the solid phase leads to an uncorrelated statistical distribution of particles, corresponding to a constant value of the RDF equal to 1.

Figure 11(b) and (c) show the averaged normal relative velocity between two approaching particles $\langle dv_n^- (r) \rangle$, and the collision kernel $\kappa(r)$. This collision kernel (Sundaram & Collins 1997) is obtained as the product of the RDF$(r)$ and $\langle dv_n^- (r) \rangle$:

$$\kappa(r) = \text{RDF}(r) \cdot |\langle dv_n^- (r) \rangle|,$$

(14)
when $r = 2a$. In the figure, we display the behavior of this observable with the distance $r$, which can be interpreted as the approach rate of particle pairs at distance $r$. The normal relative velocity of a particle pair is obtained as the projection of the relative velocity in the direction of the distance between the two interacting particles

$$dv_n(r_{ij}) = (\mathbf{u}_i - \mathbf{u}_j) \cdot \frac{(\mathbf{r}_i - \mathbf{r}_j)}{|(\mathbf{r}_i - \mathbf{r}_j)|} = (\mathbf{u}_i - \mathbf{u}_j) \cdot \frac{r_{ij}}{|r_{ij}|}$$

(15)

(where $i$ and $j$ denote the two particles). This scalar quantity can be either positive (when two particles depart from each other) or negative (when they approach). Hence, the averaged normal relative velocity can be decomposed into $\langle dv_n(r) \rangle = \langle dv_n^+(r) \rangle + \langle dv_n^-(r) \rangle$. To estimate the probability of a collision, i.e. the collision kernel $\kappa(r)$, the mean negative normal relative velocity is therefore needed.

It is shown in figure 11(b) that the absolute value of $\langle dv_n^-(r) \rangle$ increases with $r$ when $R \leq 10$. Particle pairs are more likely to approach with higher speeds when further away. This increase of $|\langle dv_n^-(r) \rangle|$ with $r$ is less pronounced for $R = 10$, which can be explained recalling that, in this case, there is a significant accumulation in the region around the centerline where the particles are transported downstream at almost constant velocity. When $R = 100$, $|\langle dv_n^-(r) \rangle|$ is constant and equal to 0.022. In a dense gaseous regime, particles are, on average, uniformly distributed and approach each other at similar speeds and at different radial locations: their motion is uncorrelated.

The collision rate is mainly determined by the averaged normal relative velocity when $R = 100$. As shown in figure 11(c), $\kappa(r)$ is approximately constant at different radial distances, showing slightly larger values near contact, $r = 2a$. In the cases with $R = 1$ and 10, $\kappa(r)$ is determined at small separations $r$ by the particle clustering and by the normal relative velocities at higher separations. When shear-induced migration occurs, $R = 10$, the collision kernel $\kappa(r)$ is higher than in the case of neutrally buoyant particles for separations between 2 and 3 particle radii. When $r \gtrsim 3$ the Radial Distribution Function drops to 1 and the approach rate is therefore determined by the averaged normal relative velocity. Since the absolute value of $|\langle dv_n^-(r) \rangle|$ grows more slowly with $r$ for $R = 10$, $\kappa(r)$ shows the same trend.

Before concluding the section, we examine the collision statistics when increasing the volume fraction $\phi$ while keeping the mass fraction $\chi$ constant. To this aim, we show in figure 12 the radial distribution function RDF, the averaged normal relative velocity and the collision kernel from 3 of the cases at constant mass fraction previously discussed: $\phi = 2\%$ and $R = 10$; $\phi = 5\%$ and $R = 4$; $\phi = 20\%$ and $R = 1$.

The small-scale clustering increases as the volume fraction $\phi$ increases, see figure 12(a), i.e. the RDF at $r = 2$ is highest for the flow with $\phi = 20\%$. However, as the excluded volume increases with $\phi$, the mean distance between the particles is reduced and these approach each other on average with a smaller
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relative velocity, as shown by the reduction in \( \langle dv_n^{-} (r) \rangle \) at higher \( \phi \) in the inset of figure 12(a). Finally, figure 12(b) reveals that also at constant \( \chi \) the collision rate is mainly governed by the averaged normal relative velocity. We observe indeed that \( \kappa(r) \) is higher in the most dilute cases and the data scale with the volume fraction.

4. Final remarks

We study the effect of varying solid to fluid density ratio and volume fraction in a turbulent channel flow laden with finite-size rigid spheres in the semi-dilute regime. The numerical simulations do not include the effect of gravity to disentangle the role of fluid and particle inertia, as well as of the excluded volume on the mean and fluctuating fluid velocities and particle motion.

The main finding of the work is that variations of the volume fraction have a larger impact on the statistics of fluid and solid phases than modifications of the density ratio \( R \). Indeed, we show that, when the volume fraction is kept constant \( (\phi = 5\%) \) and the density ratio, \( R \), increased from 1 to \( R \leq 10 \), the mean fluid velocity and velocity fluctuation profiles are only slightly affected. The main effect of increasing the density ratio (up to \( R = 10 \)) is the change of the mean local volume fraction, i.e. the wall-normal particle distribution across the channel. At \( R = 10 \), we report a significant shear-induced migration toward the centerline. This is shown to be an inertial effect induced by the particle density, \( R \), and the presence of a wall.

When the volume fraction is changed and either the mass fraction or the density ratio kept constant, instead, the flow statistics vary significantly. The mean streamwise velocity profiles in outer units show lower values closer to the walls and higher values toward the centerline. In inner units, the difference is even more evident, showing a continuous variation of the von Kármán constant and of the additive coefficient of the log-law, see also Picano et al. (2015) for
comparisons at constant $R = 1$. The increase in overall drag found when varying the volume fraction is considerably higher than that obtained for increasing density ratios at same volume fraction.

We also consider cases at same $\phi = 5\%$ and $R = 100$. At this high $R$, the motion of the solid phase decouples from the dynamics of the fluid phase and the statistics drastically change. The particles are uniformly distributed across the channel and behave as a dense gas with uniform mean streamwise velocity and uniform isotropic velocity fluctuations across the channel. The dense gas behavior of the solid phase clearly emerges in the probability density function of the modulus of the velocity fluctuations that closely follows a Maxwell-Boltzmann distribution. The fluid velocity fluctuations are reduced and are almost constant except in the regions close to the walls. For $R = 100$ we also find that the streamwise dispersion is one or two orders of magnitude smaller than in the cases at lower $R$. In channel flows, the streamwise particle dispersion is enhanced by the inhomogeneity of the mean velocity profile. However as we have shown, at very high density ratios this inhomogeneity is lost leading to a reduction of the mean streamwise particle displacement.

Finally, we have examined the radial distribution of particles and their collision kernel. For $1 \leq R \leq 10$ and constant $\phi = 5\%$, the collision rate is mostly controlled by the particle clustering near contact. Instead, for $R = 100$, the number of collisions is enhanced and essentially determined by the particle average normal relative velocity. For suspensions at fixed mass fraction $\chi = 0.2$, the collision rate decreases with increasing $\phi$.

Our results therefore suggest that the particle motion in the absence of gravity is not significantly different between neutrally buoyant particles and heavy particles with density ratios typical of sediments and metal particles in liquids. The main effects on the flow statistics are due to variations of the volume fraction, thus of the excluded volume. The main effect of increasing the density ratio is the appearance of a shear-induced migration while velocity statistics are almost unchanged. The present results may help to interpret the dynamics of sediments in shear turbulence.

This work was supported by the European Research Council Grant No. ERC-2013-CoG-616186, TRITOS and from the COST Action MP1305: Flowing matter. Computer time provided by SNIC (Swedish National Infrastructure for Computing) and CINECA, Italy (ISCRA Grant FIShET-HP10CQQF77).
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Paper 3
Rheology of extremely confined non-Brownian suspensions

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We study the rheology of confined suspensions of neutrally buoyant rigid monodisperse spheres in plane-Couette flow using Direct Numerical Simulations. We find that if the width of the channel is a (small) integer multiple of the sphere diameter, the spheres self-organize into two-dimensional layers that slide on each other and the effective viscosity of the suspension is significantly reduced. Each two-dimensional layer is found to be structurally liquid-like but its dynamics is frozen in time.

Suspensions of solid objects in simple Newtonian solvents (e.g., water) can show a kaleidoscope of rheological behaviors depending on the shape, size, volume fraction ($\phi$) of the additives, and the shear-rate ($\dot{\gamma}$) imposed on the flow; see, e.g., Refs. Wagner and Brady (2009); Stickel and Powell (2005) for reviews. Suspensions can be of various types, e.g., suspensions of small particles (smaller than the viscous scale of the solvent), where the solvent plays the role of a thermal bath, are called Brownian suspensions (e.g. colloids) (Wagner and Brady 2009). At small $\phi$ and under small $\dot{\gamma}$, the effective viscosity of such suspensions increases with $\phi$: $\mu_{\text{eff}} \sim (5/2)\phi$ (Batchelor 1967), as derived by Einstein (1906) [See also Ref. Brady (1983) for a $d$ dimensional generalization]. In the other category are suspensions of large particles (e.g. emulsion, granular fluids etc.), where the thermal fluctuations are often negligible. Such suspensions are called non-Brownian suspensions. For moderate values of $\phi$ and $\dot{\gamma}$ non-Brownian suspensions show continuous shear-thickening, (i.e., $\mu_{\text{eff}}$ increases with $\dot{\gamma}$) (Fall \textit{et al.} 2010; Picano \textit{et al.} 2013) which can be understood (Picano \textit{et al.} 2013) in terms of excluded volume effects. Such a rheological response has been observed in many natural and industrial flows, including flows of mud, lava, cement, and corn-starch solutions. Dense (large $\phi$, close
to random close packing) non-Brownian suspensions may show discontinuous shear-thickening (Brown and Jaeger 2009; Fernandez 2013) – a jump in effective viscosity as a function of $\dot{\gamma}$.

Recent experiments have uncovered intriguing rheological behavior of dense (large $\phi$) suspensions under confinement (Fall et al. 2010; Brown and Jaeger 2009; Brown 2010). Common wisdom suggests that, under confinement, the inertial effects are generally unimportant at small $\dot{\gamma}$. However, a series of recent studies (Di Carlo 2009; Lee et al. 2010; Di Carlo et al. 2009; Amini et al. 2012) have demonstrated that the effect of fluid inertia, although small, can give rise to variety of effects even in microfluidic flows. Drawing inspirations from these two sets of works, we study the effects of confinement on non-Brownian suspensions with moderate values of $\phi$ and $\dot{\gamma}$. In particular, we choose the range of $\phi$ and $\dot{\gamma}$ such that in bulk the suspensions show continuous shear-thickening.

As a concrete example, we consider direct numerical simulations (DNS) of three-dimensional plane-Couette flow – with the $x$, $y$ and $z$ coordinates along the stream-wise, span-wise and wall-normal directions [see Fig. (1) of Supplemental Material] seeded with neutrally-buoyant rigid spheres of radius $a$. The fluid is sheared by imposing constant stream-wise velocity of opposite signs, $U_0 = \dot{\gamma}L_z/2$ at $z = \pm L_z/2$. We study the effects of confinement by changing the dimensionless ratio $\xi \equiv L_z/2a$, where $L_z$ is the channel width in the $z$ direction.

The most striking result of our simulations is that at or near integer values of $\xi$, the effective viscosity $\mu_{\text{eff}}$ decreases significantly compared to its bulk value (Fig. 1a and b). This drop can be so large that the volumetric flow rate in a thinner channel ($\xi = 2$) is more than in a wider channel ($\xi = 2.5$), see Fig. (1c). We further demonstrate that, at small integer values of $\xi$, the rigid spheres self-organize into an integer number of horizontal layers, which slide on one another, see Fig. (2). This, in turn, decreases the transport of horizontal momentum across the layers generating the drop in effective viscosity. We also show that at integer values of $\xi$, for which layers appear: (i) the movement of spheres across layers is not a diffusive process, Fig. (3), (ii) the typical residence time of the spheres in a layer is much longer than the time scale set by the shear, $\dot{\gamma}^{-1}$; in fact, a large number of spheres never leave the layer within the runtime of the simulations Fig. (4a); (iii) the layers are structurally liquid-like but dynamically very slow compared to the timescale set by $\dot{\gamma}^{-1}$, see Fig. (4).

In the numerical simulations, the fluid phase is described by solving the incompressible Navier–Stokes equations in three dimensions. Periodic boundary conditions are imposed on the two directions ($x$ and $y$ with lengths $L_x$ and $L_y$ respectively). The motion of the rigid spheres and their interaction with the flow is fully resolved by using the Immersed Boundary Method (Peskin 2002; Mittal and Iaccarino 2005; Breugem 2012). Lubrication models based on Brenner’s analytical solution and a soft-sphere collision model are used to properly reproduce the interactions among particles when the particle distance is below
Rheology of extremely confined non-Brownian suspensions

![Contour plot of the effective viscosity $\mu_{\text{eff}}/\mu_f$ as a function of $\xi$ and $Re$ for $\phi = 0.3$.](a)

![The effective viscosity $\mu_{\text{eff}}/\mu_f$ versus $\xi$ for $\phi = 0.3$ and for three different values of $Re = 1$ (red circles), 5 (blue squares) and 10 (black triangles).](b)

![The flow rate of matter (both solvent and additive) $F$ (blue squares, left vertical axis), defined in (1), and the flow-rate-per-unit-cross-section, $f$, (red circles, right vertical axis) as a function of $\xi$, for $Re = 5$ and $\phi = 0.3$.](c)

**Figure 1.** (a) Contour plot of the effective viscosity $\mu_{\text{eff}}/\mu_f$ as a function of $\xi$ and $Re$ for $\phi = 0.3$. (b) The effective viscosity $\mu_{\text{eff}}/\mu_f$ versus $\xi$ for $\phi = 0.3$ and for three different values of $Re = 1$ (red circles), 5 (blue squares) and 10 (black triangles). (b) The flow rate of matter (both solvent and additive) $F$ (blue squares, left vertical axis), defined in (1), and the flow-rate-per-unit-cross-section, $f$, (red circles, right vertical axis) as a function of $\xi$, for $Re = 5$ and $\phi = 0.3$.

In practice, we change $L_z$ but hold the particle radius $a$ fixed. The effective viscosity, $\mu_{\text{eff}}$, is thus function of the dimensionless numbers, $\phi$, $\xi$ and the particle Reynolds number, $Re \equiv \rho \dot{\gamma} a^2 / \mu_f$, where $\rho$ and $\mu_f$ are the density and dynamic viscosity of the solvent. The size of the rectangular box is $16a \times 16a$ in the streamwise and spanwise directions. The Cartesian mesh uses 8 grid points per particle radius $a$. The surface of each particle is discretized with 746 Lagrangian grid points.

Initially, the spheres are placed at random locations, with no overlap between each other, and with velocities equal to the local fluid velocity of the laminar Couette profile [Fig. (1) of Supplemental Material]. We calculate the effective viscosity, $\mu_{\text{eff}}$, as the ratio between the tangential stress at the walls and the mesh size (Lambert et al. 2013). A complete description of the equations and the details of the algorithm is provided as supplemental material.
The effective viscosity $\mu_{\text{eff}}$ is shown in Fig. (1a) and Fig. (1b) as a function of $Re$ and $\xi$, for $\phi = 0.3$. For large channel widths, e.g., $\xi = 5$, and large volume-fractions, e.g., $\phi \geq 0.2$, we obtain shear-thickening [see Supplemental Material Fig. (4)] as was found earlier in Ref. Picano et al. (2013).

Here we address how confinement affects the rheology. Experiments (Peyla and Verdier 2011), in agreement with earlier numerical calculations (Davit and Peyla 2008), have found that at small volume-fraction ($\phi \leq 0.15$), $\mu_{\text{eff}}$ increases as $\xi$ decreases. Our results [Supplemental Material, Fig. (4)] also support this conclusion. Furthermore, our simulations can access hitherto unstudied higher values of volume-fraction ($\phi \geq 0.2$) for which this trend seems to reverse, i.e., $\mu_{\text{eff}}$ decrease with confinement. On deeper scrutiny, a more striking picture...
emerges. As we show in Fig. (1b), for \( \phi = 0.3 \), at or near small integer values of \( \xi (\xi = 2, 3, \text{and } 4) \), the effective viscosity drops significantly. The minimum value of viscosity is found at \( \xi = 2 \), which is as low as 50% of its bulk value (\( \xi \geq 6 \)). To appreciate how dramatic this effect is, we measure the (dimensionless) flux of matter (i.e. both the fluid and the spheres) through the channel, defined as

\[
F \equiv \frac{1}{\gamma L_z a^2} \int V_z p(z) dy dz; \tag{1}
\]

where \( V \equiv \zeta U^p + (1 - \zeta) u \) (F. Picano et al. 2015), with \( \zeta = 1 \) at a grid point inside a rigid sphere but \( \zeta = 0 \) otherwise \(^1\). Here, \( U^p \) is the velocity of the sphere, \( u \) is the velocity of the fluid, \( p(z) = 1 \) for \( z \geq 0 \) and \(-1\) for \( z < 0 \), and \( \langle \cdot \rangle \) denotes averaging over time. In Fig. (1c) we report \( F \) as a function of \( \xi \). As the flux \( F \) is not normalized by the cross-sectional area of the channel it is expected to increase linearly as a function of \( \xi \). This expectation indeed holds for \( \xi > 4 \). But, below that, for integer values of \( \xi \) the effective viscosity can decrease so much that \( F \) is not even a monotonic function of \( \xi \), in particular, \( F(\xi = 2) > F(\xi = 2.5) \); the flux through a wider channel is actually smaller. The flux-per-unit-area, \( f \equiv Fa^2/(Ly Lz) \), shown in Fig. (1c) is expectedly a constant at large \( \xi \). For the small integer values of \( \xi \), it is significantly higher than its bulk value.

The drop in \( \mu_{\text{eff}} \) at integer values of \( \xi \) has been experimentally observed in Ref. Brown (2010) who studied the problem in a different parameter regime – negligible inertial and high volume fraction – where the non-confined solution shows discontinuous shear-thickening. Other experimental (Peyla and Verdier 2011) and numerical work (Davit and Peyla 2008), again in the realm of negligible inertia, have also observed some signatures of this intriguing phenomenon \(^2\) which, according to our results is an effect of inertia, missing in these earlier works.

To investigate the mechanism behind the rheology, we examine snapshots of the spheres, see Fig. (2a) for \( \xi = 2 \) (top) and \( \xi = 2.5 \) (bottom). The spheres are color-coded by their initial wall-normal locations (red corresponds to an initial position near the top boundary and blue to the bottom boundary). It can be clearly observed, that for \( \xi = 2 \), the particles form a bi-layered structure. This layering is also confirmed by the wall-normal profiles of the average particle volume fraction, \( \rho_p(z) \equiv \langle \zeta(x, y, z, t) \rangle_{x, y, t} \), displayed in Fig. (2b) for \( \xi = 2, 2.5 \) and 3. In the first and the last case, one can observe equally-spaced two and three prominent peaks respectively. Note that a weaker layering is

\(^1\)The phase indicator \( \zeta \) is is related to the volume fraction by \( \phi = (1/V) \int \zeta dV \) where \( V \) is the total volume of the channel.

\(^2\) The experimental data reported in Ref. Peyla and Verdier (2011) is for small to moderate values of \( \phi \). At the higher value of \( \phi \) (around 0.2) the authors find some signatures of non-monotonic behaviour. But the data were fitted with a monotonic function, probably motivated by their earlier numerical study (Davit and Peyla 2008). Further, the apparent minimum observed in the numerical data for effective viscosity in Ref. Davit and Peyla (2008) seems to occur at a half-integer value of the confinement parameter for one value of \( \phi \) and seem to disappear at a higher value of \( \phi \).
Figure 3.  (a) The PDF, $P(d_z)$, of the displacement ($d_z$) of the center of the spheres along the $z$ direction for $\xi = 2$, at early times, $t = 2.5\dot{\gamma}^{-1}$ (red, filled triangles) and late times $t = 386\dot{\gamma}^{-1}$ (red, open triangles) for $Re = 5$. For comparison, the inset shows the PDF, $P(d_y)$, of the displacement ($d_y$) along the $y$ direction at early times, $t = 2.5\dot{\gamma}^{-1}$ (black, filled diamonds) and moderate times $t = 5\dot{\gamma}^{-1}$ (black, open diamonds). (b) Log-log plot of mean square displacement of the spheres, $S_z^2$, versus $t\dot{\gamma}$. The curves have been translated in the $y$–direction for clarity. At late times, $S_z^2 \sim t^\beta$, where $\beta = 1$ implies diffusion. For three different values of $\xi = 2$ (red triangles), 2.5 (blue squares) and 3 (black dots), we obtain $\beta \approx 0.61$, 0.95 and 0.88, respectively. (c) The PDF, $P(d_z)$, of the displacement ($d_z$) of the center of the spheres along the $z$ direction for $\xi = 2.5$. The PDF of $d_y$, $P(d_y)$, is shown in the inset.

observed for $\xi = 2.5$. The drop in effective viscosity thus corresponds to the formation of layers that slide on each other, with little transport of momentum across the layers. For $\xi = 2$, where layering is most prominent, the particles form disordered liquid-like structures, within each layer, as seen by the radial distribution function of the position of the spheres, see Supplemental Material,
Fig. (7). Within a layer, the each sphere does not simply slide with the flow but also show rolling, see Supplemental Material, Fig. (9).

In order to understand the dynamics of particles in the wall-normal direction, we show in Fig. (3a), the probability distribution function (PDF) of the displacement of the spheres, $d_z(t) \equiv z_c(t) - z_c(0)$, at different times, where $z_c(t)$ is the $z$ coordinate of the center of a sphere. Obviously, as $t \to 0$ the PDF $[P(d_z)]$ must approach a Dirac delta function. Remarkably, for $\xi = 2$ the PDF has exponential tails, i.e., it is non-diffusive, with some particles undergoing larger displacements as shown in Fig. (3a). At later times, for $\xi = 2$, the PDF of $d_z$ develops a peak at $d_z/(L_z - 2a) = 1$, indicating the hop between two layers. A similar behavior is observed for $\xi = 3$ too. Contrast this result with the PDF of the displacement along the span-wise($y$) direction, inset of Fig. (3a), which
clearly shows Gaussian behavior at all times, implying diffusive dynamics. The second moment of these PDFs provides the mean squared displacement of the particles, \( S_z^2(t) = \langle [z_c(t) - z_c(0)]^2 \rangle_p \), the time evolution of which is shown in Fig. (3b). At late times, in general, a power-law dependence on time is found, \( S_z^2(t) \sim t^\beta \), where \( \beta = 1 \) would imply a simple diffusive behavior. For \( \xi = 2, 3 \) we estimate \( \beta \approx 0.61 \) and 0.88 respectively. But for \( \xi = 2.5, \beta \approx 1 \) is obtained. The diffusive behaviour for \( \xi = 2.5 \) can be further confirmed by plotting the PDF of \( d_z \). At intermediate times \( (t = 2.5\hat{\gamma}^{-1}) \), for \( \xi = 2.5 \), the PDF develops Gaussian tails, indicative of a diffusive process and at late times it approaches a constant see Fig. (3c)]).

To visualize the dynamics, we provide movies of the particles’ trajectories (available at https://www.youtube.com/watch?v=Qn4DiXZFsbw for the case \( \xi = 2 \) and at https://www.youtube.com/watch?v=AmNsAsYoec8 for the case \( \xi = 2.5 \) ). These clearly demonstrate that for \( \xi = 2 \), each horizontal layer is structurally disordered but dynamically frozen (i.e. the particle motion relative to the layer is dynamically frozen). We quantify this phenomenon by three different measurements:

(A) We calculate the residence time (\( \tau \)) of a sphere in a single layer. The residence time is defined as \( \tau = \max \{t|d_x(t) < \pm a\} \). Instead of calculating the PDF by histograms of \( \tau \), we calculate the cumulative PDF, \( Q(\tau) \), by the rank-order method (Mitra et al. 2005), as the latter is free from binning errors. The cumulative PDF, \( Q(\tau) \), is displayed in Fig. (4a) as a function of \( \tau \) for \( \xi = 2 \) and 2.5 for \( Re = 1 \) and 5. For \( \xi = 2, Q \) remains very close to unity during the whole duration of the simulation, i.e., very few spheres actually move from one layer to another. In other words, the layers are quite stable to perturbations in wall-normal directions. Conversely for \( \xi = 2.5 \), \( Q(\tau) \) can be fitted by a Gaussian.

(B) The streamwise velocity auto-correlation function of the spheres, \( R_{xx} \equiv \langle U_p^x(t)U_p^x(0) \rangle \), is shown in Fig. (4b). For \( \xi = 2 \), \( R_{xx} \approx 1 \) for a very long time, implying that the temporal fluctuations of the stream-wise velocity are negligible. This suggests that each sphere moves in a layer with a uniform stream-wise velocity keeping their relative distances practically constant. For the cases where the layering is not very strong, e.g., \( \xi = 2.5 \) the auto-correlation function decays rapidly. For \( \xi = 3 \), layering reappears and \( R_{xx} \) again shows slow decay in time.

(C) Let us define \( r_{\|}(t; r_0) \) to be the horizontal distance between a pair of spheres at time \( t \), which were at a distance \( r_0 \) at \( t = 0 \) (and in the same layer). If the layers formed by the spheres were truly frozen-in-time we would obtain \( r_{\|}(t; r_0) = r_0 \) for all \( t \) and \( r_0 \). In Fig. (4c), we show the time evolution of \( \langle r_{\|}^2(t; r_0) \rangle_p \), for \( r_0 = 4a \), where the symbol \( \langle \cdot \rangle_p \) denotes averaging over all possible particle pairs.\(^3\) Had the spheres moved chaotically within a layer, \( r_{\|} \)
would have grown exponentially with time. Clearly for all the cases shown in Fig. (4c), $r_{\parallel}$ grows at most linearly with time. In particular, when layering occurs ($\xi = 2, 3$), it takes a long time ($t \geq 430 \gamma^{-1}$) for $r_{\parallel}(t; 4a)$ to grow by a factor of two. This quantifies again the dynamical stability of the layer, the relative in-plane distance between pairs of spheres change slowly (linearly) with time.

In conclusion, using numerical simulations, we demonstrate that the effective viscosity of an extremely confined non-Brownian suspension can exhibit a non-monotonic dependence on the channel width, in particular the effective viscosity sharply decreases if the channel width is an (small) integer multiple of particle diameter. We demonstrate that this behavior is accompanied by a change in micro-structure, namely the formation of particle layers parallel to the confining plates. The two-dimensional layers formed by the particles slide on each other, the layers are structurally liquid-like by evolve on very slow time scales. Similar layering under shear, have been theoretically anticipated (Zurita-Gotor et al. 2012; Katz 2014), but the consequences for transport in extreme confinement as shown by us has never been demonstrated before. We finally note that our results are in contrast with the case of sheared Brownian suspensions where the structures were found to be uncorrelated with measured viscosity (Xu et al. 2012). Note also that recent studies (Thiébaud et al. 2014; Kaoui et al. 2014) have found anomalous rheological behavior in confined suspension of vesicles (and capsules) where also the self-organization of the capsules into files is observed. In such suspensions, the deformability and the non-sphericity of the capsules are also expected to play a role.

1. Acknowledgment

LB and WF acknowledge financial support by the European Research Council Grant No. ERC-2013-CoG-616186, TRITOS and computer time provided by SNIC (Swedish National Infrastructure for Computing). DM acknowledges financial support from Swedish Research Council under grant 2011-542 and 638-2013-9243. PC thanks NORDITA for hospitality.

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We study extremely confined suspensions of neutrally-buoyant rigid and spherical particles in shear flow. A sketch of the plane-Couette flow with the coordinate system used is presented in Fig. (5). The analysis focuses on the variation of the channel gap, \( L_z \). In the main manuscript, \( L_x \) and \( L_y \) denote the streamwise and spanwise lengths of the computational domain.

1.2. Direct numerical simulation

Simulations have been performed using the numerical code originally described in Ref. [17] that fully describes the coupling between the solid and fluid phases. The Eulerian fluid phase is evolved according to the incompressible Navier-Stokes equations,

\[
\nabla \cdot \mathbf{u} = 0
\]

\[
\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{u} + \mathbf{f}
\]

where \( \mathbf{u} \), \( \rho \) and \( \nu = \mu/\rho \) are the fluid velocity, density and kinematic viscosity respectively (\( \mu \) is the dynamic viscosity), while \( p \) and \( \mathbf{f} \) are the pressure and a generic force field (used to model the presence of particles). The particles centroid linear and angular velocities, \( \mathbf{U}_p \) and \( \mathbf{\Omega}_p \) are instead governed by the Newton-Euler Lagrangian equations,

\[
\rho_p V_p \frac{d\mathbf{U}_p}{dt} = \rho \oint_{\partial V_p} \tau \cdot \mathbf{n} \, dS
\]

\[
\mathcal{I}_p \frac{d\mathbf{\Omega}_p}{dt} = \rho \oint_{\partial V_p} \mathbf{r} \times \tau \cdot \mathbf{n} \, dS
\]

where \( V_p = 4\pi a^3/3 \) and \( \mathcal{I}_p = 2\rho_p V_p a^2/5 \) are the particle volume and moment of inertia; \( \tau = -p\mathbf{I} + 2\mu \mathbf{E} \) is the fluid stress, with \( \mathbf{E} = (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)/2 \) the deformation tensor; \( \mathbf{r} \) is the distance vector from the center of the sphere while \( \mathbf{n} \) is the unity vector normal to the particle surface \( \partial V_p \). Dirichlet boundary conditions for the fluid phase are enforced on the particle surfaces as \( \mathbf{u}|_{\partial V_p} = \mathbf{U}_p + \mathbf{\Omega}_p \times \mathbf{r} \).

**Figure 5.** Sketch of the flow configuration and adopted coordinate system.
An immersed boundary method is used to couple the fluid and solid phases. The boundary condition at the moving particle surface is modeled by adding a force field on the right-hand side of the Navier-Stokes equations. The fluid phase is therefore evolved in the whole computational domain using a second order finite difference scheme on a staggered mesh while the time integration is performed by a third order Runge-Kutta scheme combined with a pressure-correction method at each sub-step. This integration scheme is also used for the Lagrangian evolution of eqs. (4) and (5). Each particle surface is described by uniformly distributed $N_L$ Lagrangian points. The force exerted by the fluid on the particles is imposed on each $l$-th Lagrangian point. This force is related to the Eulerian force field $f$ by

$$f(x) = \sum_{l=1}^{N_L} F_l \delta^3(x - X_l) \Delta V_l$$

where $\Delta V_l$ is the volume of the cell containing the $l$-th Lagrangian point while $\delta^3$ is the three dimensional Dirac delta distribution. The force field is calculated through an iterative algorithm that ensures a second order global accuracy in space. In order to maintain accuracy, eqs. (4) and (5) are rearranged in terms of the IBM force field,

$$\rho_p V_p \frac{dU_p}{dt} = -\rho \sum_{l=1}^{N_L} F_l \Delta V_l + \rho \frac{d}{dt} \int_{V_p} u \, dV$$

$$I_p \frac{d\Omega_p}{dt} = -\rho \sum_{l=1}^{N_L} r_k \times F_l \Delta V_l + \rho \frac{d}{dt} \int_{V_p} r \times u \, dV$$

where $r_k$ is the distance from the center of a particle. The second terms on the right-hand sides are corrections to account for the inertia of the fictitious fluid contained inside the particles.

Lubrication models based on Brenner asymptotic solution are used to correctly reproduce the interaction between two particles when the distance between them is smaller than twice the mesh size. Denoting the distance between the two particles normalized by the radius $a$ as $\epsilon$, the lubrication correction for two equal spheres in squeezing motion is expressed as

$$F_{lc} = -6 \pi \mu f a \ u_s [\lambda(\epsilon) - \lambda(\epsilon_{lc})]$$

where $u_s$ is half the relative velocity between the two spheres (along their line of centres), and $\epsilon_{lc}$ is the threshold distance at which the lubrication correction is activated. In equation 8, $\lambda(\epsilon)$ is the asymptotic expansion of Brenner’s analytical solution:

$$\lambda(\epsilon) = \frac{1}{2\epsilon} - \frac{9}{20} \log \epsilon - \frac{3}{56} \epsilon \log \epsilon + 1.346 + O(\epsilon),$$

For the squeezing motion between a particle and a wall, a different asymptotic expansion is used,

$$\lambda(\epsilon) = \frac{1}{\epsilon} - \frac{1}{5} \log \epsilon - \frac{1}{21} \epsilon \log \epsilon + 0.9713 + O(\epsilon),$$

while equation 8 is modified substituting $u_s$ with the particle normal velocity toward the wall.
These lubrication corrections would diverge when $\epsilon \to 0$. They are therefore turned off below a threshold distance ($\epsilon_t = 0.001$) since it is known from experiments that collisions actually occur between particles and particles and walls. A soft-sphere collision model is used to account for collisions. In this model, particles are allowed to slightly overlap with each other and the solid contact force is computed from the overlap between the particles and their relative velocity. The collision time is artificially stretched on $N_c = 8$ computational time steps to avoid severe constraints on the numerical time step. An almost elastic rebound is ensured with a restitution coefficient set at 0.97. This is the typical coefficient of restitution measured from dry collisions between two rigid spheres.

These lubrication and collision forces are added to the right-hand side of eq. (6). The code has been validated against several classic test cases [17,18] and has been used earlier to study shear-thickening in inertial suspensions, see Ref. [7].

1.3. Measurement of effective viscosity

We calculate the effective viscosity as the ratio between the tangential stress at the walls and $\dot{\gamma}$. The tangential stress, and consequently the effective viscosity, is different at different points of the wall and also at each point changes as a function of time. At each time, we calculate the average of this effective viscosity over the walls and obtain a time-series $\mu_{\text{eff}}(t)$. This time-series is displayed in Fig. (6) for one particular case. Clearly, after a short while the effective viscosity reaches a stationary value with fluctuations about it. Typically, we find that our simulations reach statistically stationary state when time $t \geq 200 \dot{\gamma}^{-1}$.

The average of $\mu_{\text{eff}}(t)$ over this statistically stationary state is the effective viscosity $\mu_{\text{eff}}$ while the standard deviation of the fluctuations is used as an estimate of the error in the measurement of $\mu_{\text{eff}}$. These are reported in Table 1. A careful look at the table will convince the reader that the relative strength of the fluctuations decreases at commensuration. The effective viscosity $\mu_{\text{eff}}$ is also shown in Fig. (7).

1.4. Effective viscosity as a function of volume fraction

We depict the variation of the effective viscosity, $\mu_{\text{eff}}$, as a function of the volume fraction, $\phi$, in Fig. (8) and as a function of confinement, $\xi$, in Fig. (9). Clearly the non-monotonic behavior of $\mu_{\text{eff}}$ vanishes as $\phi$ is reduced.

1.5. Three dimensional view of particle position for $\xi = 3$

To complete the analysis in the manuscript, we display three dimensional views of the particle positions in Fig. (10) for $Re = 5$, $\phi = 0.3$ and $\xi = 3$. The top and bottom images are taken $150 \dot{\gamma}$ and $870 \dot{\gamma}$ time units after an initial reference time at statistically steady state. The particles stay in layers for longer times for $\xi = 3$ than for $\xi = 2.5$ as shown by the streamwise auto-correlation function and by the averaged squared relative distance between pair of spheres displayed in the manuscript. The particles are mixed only after a relatively long time.
Re = 1. When compared with the data in the paper, this figure reveals and shows that the radial distribution function of the position of the centers of the spheres in the x–y plane is shown in Fig. (11). This is defined as

\[ R_{\parallel} \equiv \frac{1}{2\pi r Dz n_0} \frac{dN_r}{dr} \]  

(11)

where \( N_r \) is the number of particles in a cylinder of radius \( r \) and \( n_0 = N_p(N_p - 1)/(2V) \) is the density of particle pairs in a volume \( V \) with \( N_p \) the total number of particles.

1.6. In-layer radial distribution function

The radial distribution function of the position of the centers of the spheres in the x–y plane is shown in Fig. (11). This is defined as

\[ R_{\parallel} \equiv \frac{1}{2\pi r Dz n_0} \frac{dN_r}{dr} \]  

(11)

where \( N_r \) is the number of particles in a cylinder of radius \( r \) and \( n_0 = N_p(N_p - 1)/(2V) \) is the density of particle pairs in a volume \( V \) with \( N_p \) the total number of particles.

1.7. Streamwise auto-correlation function for \( Re = 1 \)

In Fig. (12) we show the streamwise particle auto-correlation function \( R_{xx} \) for \( Re = 1 \). When compared with the data in the paper, this figure reveals and shows that the radial distribution function of the position of the centers of the spheres in the x–y plane is shown in Fig. (11). This is defined as

\[ R_{\parallel} \equiv \frac{1}{2\pi r Dz n_0} \frac{dN_r}{dr} \]  

(11)

where \( N_r \) is the number of particles in a cylinder of radius \( r \) and \( n_0 = N_p(N_p - 1)/(2V) \) is the density of particle pairs in a volume \( V \) with \( N_p \) the total number of particles.
Figure 6. The effective viscosity $\mu_{\text{eff}}(t)$ (normalized by the viscosity of the solvent) as a function of time for one representative run.

confirms the importance of inertial effects. The streamwise autocorrelation decays faster for $Re = 1$ than for $Re = 5$, because, at higher $Re$, the particles are more constrained to move in the same direction of the carrier flow. This is more evident for $\xi = 3$. 
Figure 7. Surface plot of the effective viscosity $\mu_{\text{eff}}$ as a function of $\xi$ and $Re$ for $\phi = 0.3$. The inset shows $\mu_{\text{eff}}/\mu_{f}$ versus $\xi$ for $\phi = 0.3$ and for three different values of $Re = 1$ (red circles), 5 (blue squares) and 10 (black triangles).

Figure 8. The effective viscosity $\mu_{\text{eff}}/\mu_{f}$ versus $\phi$ for two different values of $Re = 1$ (dashed lines) and 5 (continuous lines) for three different values of $\xi = 1$ (black filled circles), 2 (blue squares) and 5 (red triangles).
Figure 9. The effective viscosity $\mu_{\text{eff}}/\mu_f$ versus the confinement $\xi$ for $\phi = 0.05$ (red diamonds), 0.2 (black squares) and 0.3 (blue filled circles).

Figure 10. Three dimensional view of positions of the spheres for $Re = 5$, $\phi = 0.3$ and $\xi = 3$ at $150\dot{\gamma}$ and $870\dot{\gamma}$ time units after an initial reference time. The particles are color coded by their initial wall-normal position. (red: close to the top boundary, blue: close to the bottom boundary).
Figure 11. The radial distribution function of the position of the centers of the spheres in the $x-y$ plane.

Figure 12. Streamwise velocity auto-correlations for $Re = 1$ for $\xi = 2$ (red triangles), 2.5 (blue squares), and 3 (black dots).
Figure 13. Sliding and rolling motion of a particle for $\xi = 2$ and $Re = 5$. The red cross shows at each time the position of the centre of the sphere while the blue filled circle the position of a lagrangian point on the surface of the sphere. The wall is located at $z/a = 2$. 