Report

DNS of particle dispersion in counter-current sheared air/water flow

Author(s):
Botto, Lorenzo

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DNS of particle dispersion in counter-current sheared air/water flow.
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Abstract

Lo studio dei meccanismi di dispersione e deposizione turbolenta di gocce o particelle vicino all’interfaccia di separazione fra liquidi e gas ha notevoli risvolti applicativi in campo ambientale, in studi di geofisica e in processi industriali. I flussi termici fra atmosfera e oceano sembrano infatti essere fortemente condizionati dalla presenza di aerosol sulla superficie marina, tramite il processo di evaporazione e condensazione. La dispersione di sostanze inquinanti nell’atmosfera può essere predetta e al limite controllata. Si possono inoltre ottimizzare i processi di combustione conoscendo dove le particelle di fluido combustibile tendono a segregare, nelle vicinanze di film liquidi. Questi pochi esempi sottolineano la notevole importanza pratica di questa materia.

Tali meccanismi sono controllati dalle strutture coerenti turbolente che si formano in prossimità dell’interfaccia che separa la corrente fluida da quella gassosa. La forma e la posizione di quest’ultima e’ a sua volta determinata dalla dinamica delle due fasi. Osservazioni numeriche e sperimentali lasciano supporre che, se l’ampiezza delle onde che costituiscono l’interfaccia è sufficientemente piccola, tipica di onde capillari, la fase gassosa percepisce quella liquida come una parete liscia e rigida; le statistiche di velocità media e delle fluttuazioni turbolente confermano queste osservazioni. L’obiettivo di questo lavoro è verificare se i meccanismi di deposizione delle particelle siano o meno influenzati dalla presenza di un’interfaccia deformabile.

Ricerche fondamentali in questo campo sono state finora condotte sia con approcci sperimentali, che richiedono costose apparecchiature di visualizzazione e misura, sia con approcci computazionali, resi complicati dalle possibili interazioni fra le fasi coinvolte. Durante lo svolgimento di questa tesi è stato condotto un tracciamento Lagrangiano di gocce d’acqua micrometriche in un flusso turbo-
lento d’aria che scorre sopra una superficie che è libera di deformarsi nel tempo, con formazione di onde capillari. I risultati ottenuti sono stati confrontati con quelli relativi a un canale aperto convenzionale, in cui l’interfaccia deformabile è sostituita da una lastra piana.

Le statistiche riguardanti la distribuzione di velocità delle particelle al centro del canale non rivelano significative differenze fra i due casi. Il tasso di deposizione delle particelle sull’interfaccia deformabile è invece considerevolmente superiore a quello sulla lastra piana. Questo a sua volta determina una diversa distribuzione di concentrazione della fase dispersa in direzione ortogonale alla parete. In questa tesi è stato reso evidente, attraverso analisi quantitative, come il processo di deposizione sia costituito da due stage successivi, dominati da differenti meccanismi fisici. Attraverso un trasferimento di tipo convettivo basato sul ciclo delle sweeps e delle ejections, le particelle raggiungono il sottostato viscoso, dove si accumulano in strisce ad alta concentrazione e permangono per tempi relativamente lunghi senza depositare immediatamente. Risultati ottenuti in questo lavoro e in lavori precedenti rivelano che questo processo iniziale è molto efficiente ed è quantitativamente e qualitativamente simile nei due casi considerati. La deposizione avviene in un secondo momento, a causa di deboli e casuali fluttuazioni della velocità del fluido in direzione normale, quindi attraverso un meccanismo di tipo diffusivo; questo è stato dimostrato tramite un’analisi statistica della velocità con cui le particelle depositano. La regione vicino all’interfaccia mobile è considerevolmente più attiva in termini di intensità turbolenta della zona vicino alla lastra piana (in cui il fluido può essere considerato essenzialmente quiescente), e questo spiega l’incremento del tasso di deposizione sulla superficie deformabile. Questo è il principale meccanismo di deposizione nel caso di particelle leggere. Per particelle pesanti, meccanismi di tipo inerziale sono un contributo importante e vanno considerati.

Le analisi condotte rivelano che anche deboli differenze nelle caratteristiche delle superfici di deposizione possono avere effetti importanti sui flussi di particelle, determinando differenti tassi di deposizione e modificando la distribuzione spaziale della fase dispersa. Questo suggerisce che modelli approssimati di dispersione di particelle non possono esimersi dal considerare le specifiche caratteristiche delle superfici delimitanti il sistema fisico.
Chapter 1

INTRODUCTION

1.1 Motivations

Particle laden flows have been extensively studied in simple geometries. Nowadays, the fast growth of computational resources makes it feasible to simulate quite complex systems, even if only at low Reynolds numbers. In particular, in the last years, direct numerical simulations of turbulence in multi-phase flow systems, in which immiscible phases are interacting together through deformable interfaces, have been performed. On the contrary, a few investigations have addressed the study of the behaviour of particles and droplets moving in these flows, in spite of the variety of applications that this kind of researches could lead to.

1.2 Background

Turbulent particle dispersion commonly refers to the transport of particles within a turbulent continuous (carrier) phase. Describing the motion of dispersed phase is of great interest in several practical systems. The applications include environmental (e.g. dispersion of pollutants in the atmosphere) and geophysical studies (e.g. water droplet dispersion over the ocean), as well as industrial processes (e.g. combustion systems involving dispersed fuel particles, spray drying and cooling systems, cyclone separators, etc.). These multi-phase systems may feature mass, momentum or energy transfer between the phases,
through clearly definable interfaces. Proper prediction of particle motion in turbulent flows is not very mature as compared to single phase predictions. Due to their inertia, in fact, heavy particles subjected to external forces cannot be considered as passive scalars (e.g. temperature or dispersed chemical substances). Inertial particles therefore do not exactly follow the fluid motion. Moreover, as the particle inertia increases, the time interval over which the particle velocity is correlated with its initial velocity (particle integral time scale) increases. The resulting effect is that, when a particle is introduced into a turbulent flow, it remains trapped inside an eddy for a certain time; after that period of time, it goes under the influence of another eddy, but it’s velocity maintains “memory” of the velocity achieved while it had been evolving in the previous fluid structure. The migration of the particle through several eddies, moreover, reduces the particles residence time in each eddy and mitigates the influence of the eddy on the particle trajectory (crossing trajectory effect, [12]). This very brief overview shows how difficult the understanding of particle-laden flows could be.

Attempts to model particle dispersion dates back to the pioneering work by Taylor [57], who studied the dispersion of fluid particles in stationary, homogeneous turbulence. Many other studies, on the theoretical aspects of particle dispersion, have since then been reported in the literature ([46],[61],[63]). Most of them were confined to homogeneous, isotropic turbulence. Presently, the three-dimensional, time dependent structure of a turbulent flow field is given a lot of emphasis. In particular the objective of most recent studies is to link the dynamics of the coherent structures populating the boundary layer (for a review, see Panton [40]) to the mechanism of particle dispersion. These can be ideally divided into studies of particle deposition and particle preferential concentration.

1.2.1 Particle deposition

The particle deposition process has received considerable attention due to its numerous industrial and practical applications. One of the earliest models of deposition is the one of Friedlander and Johnstone [20], who proposed the so-called free flight theory. The essence of this model is that particles are transported by gradient diffusion to within one ‘stop-distance’ of the wall, where they ac-
quire sufficient inertia to ‘coast’ across the viscous sublayer and deposit. The theory lacked rigor but it provided an attractive physical explanation to the phenomenon of deposition. Further progress on this model was reported by Davies [13], Beal [4] and Sehmel [52]. Cleaver and Yates [9] suggested that the free-flight theory ignores the structure of the near-wall turbulence. They therefore developed a sublayer model for the turbulent deposition process, which considers that the particles are carried to the wall in “sweep” events. McLaughlin’s [37] first digital simulation has shown that the particles tend to accumulate in the viscous sublayer, by virtue of inward turbulent motions in the buffer region, confirming somehow the model proposed by Cleaver et al. Rashidi and Banerjee [44], describing an experiment where particles were released in an open-channel flow, underlined the importance of the sweep-ejection events (referred by these authors as the bursting process) in depositing and entraining the particles. Also these authors reported accumulation of particles at the wall, but they noticed that particles that fall beneath the viscous sublayer whose dimensionless radius is less than 0.5 are rarely lifted up by wall ejections. The observations of Rashidi et al. have been confirmed in another experimental work, conducted by Kaftori et al. [27]. The particle behaviour was found to be intimately related to the action of quasi-streamwise vortices populating the near wall region. According to these authors, these structures take the form of “funnel-shaped” vortices, whose characteristics were studied in a previous work [28]. The influence of the near-wall coherent structures and of the bursting process on the turbulent deposition has been confirmed also in recent direct numerical simulations ([50],[59]). Some proposals to develop deterministic models that consider near wall phenomena have been recently proposed by many authors ([17, 19, 53]), following the suggestion of Cleaver and Yates. These attempts are still unsuccessful, because both the coherent structures populating the boundary layer and the interaction of the particles with these fluid movements are not yet well understood. Brooke et al. [5], performing numerical simulation, observed that particles undergo a long lasting sideways wandering in the wall normal direction until they are trapped in the coherent quasi-streamwise vortices which bring them directly to the wall. Heavy particles are more probable to deposit while the light ones tend to accumulate in the viscous sublayer and never deposit. They found the free-
flight theory to be defective even if based on reasonable assumptions, since, at any point in the viscous sublayer, only a small fraction of the deposited particles are undergoing a free-flight. In a subsequent paper, Brooke et al. [6], analyzing statistically the population of deposited particles, noticed that most of them deposit with high velocity. This led them to conclude that the free-flight mechanism may be the most important contribution to the particle accumulation and deposition at the wall. However, they pointed out also that turbulent diffusion could became important in longer simulations than they performed. From this short literary overview of particle deposition studies, it is clear that a successful model for particle deposition cannot avoid taking into account the action of the near-wall coherent structures and related sweep-ejection cycle, but it should also consider the simplicity and physical significance of a diffusion/free-flight process.

1.2.2 Particle preferential concentration

Preferential concentration (also called particle clustering) means that the instantaneous particle concentration field is correlated with the surrounding turbulent motions. Regions of either high or low particle concentration may be associated with specific turbulent structures. The degree to which turbulent eddies can modify the instantaneous concentration field depends on the Stokes number [11], defined as the ratio of the particle aerodynamic response time to some representative time scale of the flow. Many authors have tried to quantify the degree of deviation from randomness for the particle distribution field as a function of this parameter ([18],[35],[50],[56]). The underlying idea of most of these investigations, suggested by Crowe [11], is that particles with very small Stokes numbers will simply be flow tracers so the particles should be quite randomly distributed. Very large Stokes number particles, on the other hand, will not have sufficient time in a fluid element to respond to fluctuations in its velocity and will simply pass unaffected through any turbulence structure. Particles with Stokes numbers of the order of one will respond in a more dramatic way to the turbulent motions. The studies conducted in simple free-shear flow, dominated by large-scale, two-dimensional vortices, suggest that the particles with St≈1 tend to get flung away from vortex cores and collect in rings surrounding
the vortical structure ([64]). Numerical experiments in homogeneous turbulence show that particles collect in regions of high strain rate and low vorticity; they avoid vortex cores and preferentially segregate in the saddle regions between them ([35],[55],[56]). Less work has been done on examining the particle concentration field in wall-bounded flows, dominated by fully three-dimensional turbulence structure. Experiments and simulations in this case were mainly focusing on the near wall region, where the dominant effect is the accumulation of particles in the low-speed streaks ([39, 42, 44]). Fessler et al. [18] studied the particle spatial distribution at the centreplane of a channel flow (where turbulence can be considered quasi-homogeneous). He found that the greatest preferential concentration occurs when the Stokes number based on the Kolmogorov time scale is in the order of unity, confirming the results of previous works in isotropic, homogeneous turbulence (e.g. Wang and Maxey, [62]). He pointed out, however, that determining which particle is most preferentially concentrated is a complex issue, because different particles are concentrated on different fluid time scales. Rouson and Eaton [50] recently found that particles with Stokes numbers based on the Kolmogorov scale of the order of unity are preferentially concentrated into streamwise bands. Van Harleem et al. [59], performing numerical simulation, noticed that particle interaction with free-surface turbulent structures (described in [38]), leads to preferential concentration which takes the shape of large, roughly circular regions and also regions of elongated shape in which hardly any particles are present.

The accumulation of particles in the viscous sublayer ([5, 37, 59]), is also considered a phenomenon of preferential concentration, which changes the mean rather than the instantaneous concentration distribution. From a statistical point of view, the migration of particles from the core flow to the wall has been explained through the “turbophoretic effect” ([8],[47]): the dispersed phase tend to move from zones populated by large scale eddies (and high turbulent intensity) to zones populated by small-scale structures (and weak turbulent fluctuations).

The picture of preferential concentration, however, is far less complete in wall-bounded flows than in other flow conditions (homogeneous turbulence, free shear flows), because of the wide range of scales involved.
1.3 Definition of the problem and scope of the work

With respect to the motivations delineated in Section 1.1, a multi-phase flow system has been numerically simulated in the present work. The physical problem is sketched in Figure 1.1. The gas stream is flowing on top of the liquid and the interface, separating the two immiscible phases, is free to deform under the effect of shear due to the relative motion. At the liquid surface, the interaction between surface tension and gravitational forces leads to the formation of gravity-capillary waves. The characteristics of turbulence of this two-phase flow system was extensively described by Fulgosi et al. [21] and De Angelis et al. [14]. They were mainly interested in comparing the turbulence statistics of this flow and the conventional open channel flow. The main task of the present project is introducing the dispersed phase, constituted by particles or droplets, into these two flows. These particles were tracked on the gas side of the two-phase system.

The scopes of the present work can be listed as below:

- Interfacing a pre-existing Lagrangian particle tracking code to the flow solver.
- Implementing the boundary conditions for the particle phase in the Lagrangian code.
• Validating the numerical approach by comparing the results to those found in literature.

• Studying the behaviour of the dispersed phase, focusing on the differences between the wall-bounded particle laden flow and the flow over the deformable interface.

Considering the last point, this work follows the orientation of the previous investigations, which were focusing on the continuous phase. Particular attention has been put on the deposition phenomenon, which is more likely to be affected by the presence of a deformable boundary and it is of great engineering interest.
Chapter 2

NUMERICAL FORMULATION

2.1 Direct Numerical Simulation of the flow

The physical situation simulated has already been introduced in Section 1.3. The geometry of both subdomains (gas side and liquid side) is depicted in Figure 2.1. In both subdomains the fluid stream flows in the $x$ direction. For the flow over the deformable interface, hereinafter referred to as FDI, the Navier-stokes equations were solved by use of a Fourier-Chebychev, pseudo-spectral method, employing a fractional time step scheme, as discussed below. The numerical details are presented here in a very synthetic form since the simulation of the continuous phase is not the object of the current work. For further explanations the reader can refer to Fulgosi et al. ([21]) and to De Angelis et al. ([14]). The simulation of the wall-bounded flow, hereinafter referred to as OCH, has been performed following the same methodology described in [32]. In the following the three velocity components in streamwise, spanwise and normal directions will be referred to as $u$, $v$, $w$ respectively. The corresponding spatial coordinates are $x$, $y$, $z$. 
2.1.1 Governing equations for the flow

The flow in each phase is described by the momentum and continuity equations with the assumption that the fluid is incompressible, isothermal and Newtonian.

The equations are:

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

\[ \rho \frac{D \mathbf{u}}{Dt} = -\nabla p + \mu \nabla^2 \mathbf{u} + \rho g \]

Splitting the pressure into hydrostatic and hydrodynamic parts \([40]\), the generic \(i\)-component of the momentum equation can be rewritten as

\[ \frac{\partial u_i}{\partial t} + \mathbf{u} \cdot \nabla u_i = -\frac{1}{\rho} \frac{\partial \hat{p}}{\partial x_i} + \nu \nabla^2 u_i \]

where \(\hat{p}\) is the hydrodynamic pressure.

Due to the incompressibility of the flow, the second term in the left-hand-side of the previous equation, can be rewritten as,

\[ \mathbf{u} \cdot \nabla u_i = u_j \frac{\partial u_i}{\partial x_j} = \frac{\partial}{\partial x_j} (u_i u_j) \]

so that equation (2.3) can be recast in the form

\[ \frac{\partial u_i}{\partial t} = S_i - \frac{1}{\rho} \frac{\partial \hat{p}}{\partial x_i} + \nu \nabla^2 u_i \]

with \(S_i = -\frac{\partial}{\partial x_j} (u_i u_j)\) denoting the non-linear convective terms.
Continuity and momentum equations are made non-dimensional using the following flow characteristics:

- The friction velocity \( u_\star \) as a characteristic velocity
- The half height of the domain \( h \) as a characteristic length

The friction velocity is defined by

\[
u_\star = \sqrt{\frac{\tau_{\text{int}}}{\rho}}\]

where \( \tau_{\text{int}} \) is the mean shear stress at the interface.

In non-dimensional form the governing equations read:

\[
\nabla \cdot \textbf{u}^+ = 0 \tag{2.6}
\]

\[
\frac{\partial \textbf{u}^+}{\partial t^+} = \textbf{S}^+ - \nabla \hat{p}^+ + \frac{1}{Re_\star} \nabla^2 \textbf{u}^+ \tag{2.7}
\]

where the shear Reynolds number is \( Re_\star = \frac{u_\star h}{\nu} \) and its value is 85.5 for both gas and liquid.

### 2.1.2 Boundary conditions

In the absence of mass transfer, the two phases are coupled at the interface by imposing the continuity of velocities and shear stresses.

The interfacial jump conditions can then be expressed as follows:

\[
\begin{align*}
\frac{1}{Re_\star} \left( \left( \tau_{\text{L}}^+ - \tau_{\text{G}}^+ \right) \cdot \textbf{n} + \hat{p}_{\text{G}}^+ - \hat{p}_{\text{L}}^+ + \frac{1}{We} \nabla^+ \cdot \textbf{n} - \frac{1}{Fr} f^+ \right) = 0 \\
\left( \left( \tau_{\text{L}}^+ - \tau_{\text{G}}^+ \right) \cdot \textbf{t}_i \right) = 0, \quad i = 1, 2 \\
u_{\text{G}}^+ = \frac{u_\star}{Fr}
\end{align*}
\tag{2.8}
\]

where the subscripts \( L \) and \( G \) stand for liquid and gas respectively, \( \tau^+ \) is the viscous stress tensor, \( \hat{p}^+ \) is the dynamic pressure, \( f^+ \) measures the vertical displacement of the interface with respect to the mid plane, and \( \textbf{n} \) and \( \textbf{t}_i \) are the normal and the two tangential unit vectors, respectively.

The Weber (\( We \)) and Froude (\( Fr \)) numbers are defined as

\[
We = \frac{\rho_L h u_{\star L}^2}{\sigma}, \quad Fr = \frac{u_{\star L}^2 \rho_L}{g h (\rho_L - \rho_G)}
\tag{2.9}
\]

where \( \sigma \) stands for the surface tension.
The density ratio between the two phases is such that \( R = \sqrt{\frac{\rho_L}{\rho_G}} = 29.9 \), corresponding to air–water flows at atmospheric pressure and at roughly 320 K.

At the outer boundaries free–slip conditions are employed.

\[
\frac{\partial u_G^+}{\partial z^+} = \frac{\partial v_L^+}{\partial z^+} = w_G^+ = \frac{\partial p_G^+}{\partial z^+} = 0, \quad i = G, L
\]  
(2.10)

Periodic boundary conditions are used in the streamwise \((x)\) and in the spanwise \((y)\) directions.

### 2.1.3 Fractional time step technique

A modification of the fractional time step method introduced by Temam [58] is used. Equations [2.6] and [2.7] are solved together with boundary conditions alternating between gas and liquid. The time step \([\Delta t = t^{n+2} - t^n]\) is splitted in two parts: \(\Delta t_G = t^{n+1} - t^n\) and \(\Delta t_L = t^{n+2} - t^{n+1}\). In the first half of the time step \(\Delta t_G\), the governing equations are solved in the gas domain, imposing continuity of the interfacial velocity field (as calculated from the last half-step in the other subdomain). In the second half of the time step \(\Delta t_L\), the liquid flow is calculated, with continuity of interfacial shear stress imposed as a boundary condition.

### 2.1.4 Interface motion

The evolution of the interface was computed by solving a pure convection equation accounting for its vertical elevation denoted by \(f(x, t)\):

\[
\frac{\partial f}{\partial t} + u^+ \cdot \nabla f = 0
\]  
(2.11)

Since the method cannot handle strong deformations of the interface, parameters such as the Weber and Froude number were carefully selected. On the basis of scaling arguments, these non-dimensional numbers were set equal to \(We = 5.3 \times 10^{-5}\) and \(Fr = 4.5 \times 10^{-4}\), in order to limit the amplitude and steepness of the interface to the range of capillary waves. With this parameters the wave amplitudes were in the order of \(h/100\) and the wavelength was in the order \(h\).
2.1.5 Computational domain and mapping procedure

The physical domain for each phase is transformed into a rectangular parallelepiped using a nonorthogonal mapping. The transformation is performed in the normal direction only, i.e. $\xi_1 = x, \xi_2 = y$ and $\xi_3 = z - h_l(\xi_3)f(\xi_1, \xi_2, \tau)$, with $h_l$ being a linear function accounting for the deformation. The mapping is time dependent and it is re-actualized at every time step.

The dimensions of the computational domain are $l_x = 4\pi h$, $l_y = 2\pi h$, $l_z = 2h$, respectively in the streamwise, spanwise and normal directions. In wall units (i.e. normalized by kinematic viscosity and friction velocity) the dimensions are $(l_x^+, l_y^+, l_z^+) = (1074, 537, 171)$.

The grid resolution adopted consisting of $64 \times 64 \times 65$ nodes, was found adequate to resolve all the scales of turbulence ([38]).

A non uniform distribution of collocation points is used in the normal direction, using Chebychev polynomials. Thus grid spacing varies from $\Delta z^+ = 0.10$ near the boundaries to $\Delta z^+ = 4.19$ in the domain center. Note that the metrics are equivalent between the coordinates in the mapped and physical space in the homogeneous direction, but not in the normal direction.

2.1.6 Numerical scheme

The mapped equations are solved by use of a pseudo-spectral method based on Fourier representations in the streamwise and spanwise directions and a Chebychev representation in the wall-normal (nonhomogeneous) direction. For time marching, a two-level, explicit, Adams-Bashforth scheme was employed for the nonlinear terms and an implicit Crank-Nicholson algorithm for the viscous terms.
2.2 Lagrangian particle tracking

2.2.1 General assumptions

The particles are considered to be point particles and their trajectories are calculated under the assumptions of one-way coupling without mass transfer, neglecting the influence of the particles on the fluid flow (i.e. the force exerted by the fluid on each particles is the only interaction accounted for). Collisions between the particles have also been neglected as well as particle-wall interaction. These assumptions are justified since the volume fraction of the particle phase is small, i.e. the suspension is dilute. Previous works ([26, 31]) proved that turbulence modification by the particles for this class of suspensions is negligible.

2.2.2 The Lagrangian particle tracking module

A Lagrangian particle tracking code has been used to track particles in the flow field. Modifications of the original code have been made to implement the boundary conditions for the dispersed phase and to extract data of relevance to this work. The code interpolates fluid velocities from discrete grid nodes onto the particle position. With this velocity the equation of motion of the particle is integrated in time.

The code incorporates linear, cubic and fifth-order Lagrangian polynomials for interpolation yielding second, fourth, and sixth-order accuracy, respectively. For the time integration, the module has the choice between the second and fourth-order Runge-Kutta methods, and the second-order Adams-Bashforth schemes.

2.2.3 Governing equations for the particle phase

The motion of particles is described by solving a set of ordinary differential equations for the particle velocity and position at every time instant.

Most calculations found in literature are based on the Maxey and Riley [35] formulation for the force acting on a rigid sphere in a non-uniform flow under the following conditions. The diameter of the sphere is smaller than the Kolmogorov length scale and the sphere is isolated from the others and is far
from the boundaries (in this manner particle-particle interaction and particle-boundary interaction are excluded). Moreover, the Reynolds number for the relative motion between the particle and the fluid has to be small.

Based on this formulation, the equation describing the particle motion can be written as:

\[
\frac{d\mathbf{u}_p}{dt} = (1 - \frac{\rho}{\rho_p}) \mathbf{g} + \frac{\rho_p}{\rho_p} \frac{D\mathbf{u}}{Dt} - \frac{\rho}{2\rho_p} \frac{d}{dt} (\mathbf{u}_p - \mathbf{u}) - \frac{18\mu}{\rho_p d_p^2} (\mathbf{u}_p - \mathbf{u})
\]

\[- \frac{9}{\rho_p d_p} \sqrt{\frac{\mu_f I}{\pi}} \int_0^t \frac{d/d\tau (\mathbf{u}_p - \mathbf{u})}{\sqrt{t - \tau}} d\tau \] (2.12)

where \(d/dt\) denotes the time derivative along the particle path, and \(D/Dt\) denotes the time derivative following a fluid element. \(d_p\) is the particle diameter, and \(\mu\) and \(\nu\) are the dynamic and kinematic viscosities of the fluid, respectively. The terms in the right-hand-side of the equation are referred to as buoyancy force, fluid force (due to the fluid pressure gradient and viscous stresses), added-mass, Stokes drag, and Basset forces in that order. For the case of particles much heavier than the fluid \((\rho_p/\rho \gg 1)\), Elghobashi and Truesdell[16] have shown that the only significant forces are the Stokes drag, the buoyancy, and the Basset forces. Moreover, they found that the Basset force was always an order of magnitude smaller than the drag and buoyancy forces. In the present work effects of gravity are not accounted for.

Note that other authors [37, 34] included an extra force that is the Saffmann lift force [51], that can be important near the boundaries. This force acts in the wall normal direction and has the following form:

\[
f_l = -6.46\mu d_p^2 \frac{1}{4! \left(\frac{1}{\rho}\right) \frac{du_x}{dz}} \| u_{px} - u_x \| \] (2.13)

Since this force is proportional to the streamwise velocity gradient, its contribution might be important near the interface/wall and can therefore influence the particle deposition.

McLaughlin et al. [37] have shown that this term has the effect of increasing the magnitude of the vertical velocity of the particles that are passing through the viscous sublayer. In fact, a particle that is moving rapidly towards the wall
will develop a large positive value of $u_{px} - u_x$ as a consequence of the rapid variation of $u_x$ with $z$ in the viscous sublayer. This velocity difference creates then a negative Saffman lift force that accelerates the particles towards the wall. This force may then be expected to enhance the particle deposition. But, since most of the previous works do not account for this term, it has not been included in our work either. Direct comparison with other databases is therefore possible.

With this hypothesis, the particle equation can be rewritten as:

$$\frac{d\mathbf{u}_p}{dt} = -\frac{18\mu}{\rho_p \delta_p^2} (\mathbf{u}_p - \mathbf{u}) = -\frac{(\mathbf{u}_p - \mathbf{u})}{\tau_p}$$

(2.14)

where $\tau_p$ is the particle relaxation time, which is a measure of the time required by a particle released at rest to reach velocity equilibrium with the surrounding fluid.

This form of the equation is based on the assumption that drag force on the particle can be described by the Stokes drag, i.e. the drag coefficient is expressed by this relation:

$$C_d = \frac{24 \nu}{\delta_p \mathbf{u}_p - \mathbf{u}}$$

(2.15)

where $Re_p = \frac{d\nu}{u_p - u}$ is the particle Reynolds number. The Stokes regime requires the particle Reynolds number to be always less than one. Previous calculations (e.g. [37]) show instead that $Re_p$ does not necessarily remain small, in particular for depositing particles. This is the reason why an empirical relation given by Clift et al. [10] is often used to account for the non-linear drag:

$$C_d = \frac{24}{Re_p} [1 + 0.15Re_p^{0.687}]$$

(2.16)

This is included in our scheme, too.
2.2.4 Fluid time scales and particle parameters

The choice of physical parameters for the particle phase has been considered carefully. Mainly this has been subdue to three needs:

1. We want to observe a sensible deviation in the deposition rates between the chosen sets of particles.

2. It would be interesting to see phenomena of preferential concentration both in the bulk flow and near the wall.

3. It is necessary to validate the procedure by comparing the final results with previous works.

Actually the two first objectives are strictly correlated since turbulent particle transfer and deposition are controlled by the same fluid structures that causes preferential concentration. These needs are matched if the dispersed phase responds adequately to all simulated turbulent scales.

As pointed out in the introduction (Section 1.2) particle segregation occurs when particle time constant is in the same order of fluid time constant. However, the definition of the fluid time scale is a non-trivial problem in turbulent flows. There is no single set of scales rather than a continuous spectrum of velocity and length scales which must be considered.

The near-wall region is dominated by small scales. Viscous effects are important here and a time scale based on kinematic viscosity $\nu$ and friction velocity $u_*$ (usually called inner scaling) seems to be the most appropriate in this region, i.e. :

$$\tau_{f,i} = \frac{\nu}{u_*^2}$$  \hspace{1cm} (2.17)

The outer region (out of the viscous sublayer) is populated by structures with large time scales. Here a scaling with the characteristic dimension of the domain $h$ can be adopted, i.e. :

$$\tau_{f,o} = \frac{h}{u_*}$$  \hspace{1cm} (2.18)

In the above expressions, the subscripts “$i$” and “$o$” refer to inner and outer scaling, respectively.

This rough distinction between the two sets of scales was considered by Pedinotti et al. [42] who underlined the difficulty to reproduce an experiment
with a second experiment conducted at a lower Reynolds number. If one tries to match the particle response to the inner scales between the two experiments the particle response to the outer scales is necessarily different. Another scaling, based on the Kolmogorov scales, has been recognized by many workers to be the most appropriate to observe particle clustering phenomena in the bulk flow (Hogan and Cuzzi [22]) In previous calculations, however, the most used time scale is the inner scale, because the near wall region is the most interesting for turbulence-related studies and because quantitative data for deposition is reported based on this scaling. In the current work \( \tau_{f,i} \) is adopted as the definition of the time scale of the fluid, thus the Stokes number (also known as the non-dimensional response time \( \tau_p^+ \)) is simply defined as:

\[
St = \frac{\tau_p}{\tau_{f,i}} = \frac{\tau_p u_+^2}{\nu} = \frac{d_p^2 \rho_p u_+^2}{18 \nu \rho_f \nu} \quad (2.19)
\]

In the following not only the response time but every time related quantity will be made non dimensional with the viscous time scale \( \tau_{f,i} \) (e.g. the non-dimensional time step) and indicated by the superscript “+”. If the equation of motion of the particle is made non-dimensional with the friction velocity and the kinematic viscosity, i.e. :

\[
\frac{du_p^+}{dt^+} = -\frac{(u_p^+ - u^+)}{St} \quad (2.20)
\]

it becomes evident that the Stokes number is the only parameter that controls particle dispersion if no forces other than the drag force are accounted for.

Adopting previously defined time scaling, a preliminary analysis of the flow to find out which are the energy containing scales for both the cases simulated (wall bounded flow and flow over a deformable interface), has been performed. In Figures 2.2 (a) and (b) the energy spectra of streamwise velocity fluctuations are shown. Similar distributions have been found for the other components of velocity but not reported here. This statistics are relative to points situated in the center of the domain \( (x^+ = 537, y^+ = 268) \) at different elevations (thus they are not spatially averaged). For both cases there is a sudden drop off in the energy contribution (independent of the considered height) for frequencies of \( f \approx 0.25 \) corresponding to a time scale of \( \tau_{f,\text{min}} \approx 4 \). This means that there are no energy containing eddies that have characteristic time scales below \( \tau_{f,\text{min}} \).
On the other hand the biggest resolved scales have characteristic times that

On the other hand the biggest resolved scales have characteristic times that can be evaluated considering that the large scales (in the order of the domain length) populate the region near the free surface, where the mean velocity is approximately 18 $u_*$, thus:

$$\tau_{f,max} = \frac{2\pi h}{18u_*} = 85 \quad (2.21)$$

From previous considerations, the chosen Stokes number must be between $\tau_{f,min}$ and $\tau_{f,max}$ to respond to the energy containing, resolved fluid structures in the flow field.

Years of studies on particle deposition suggest that according to non-dimensional particle response times three different regimes of deposition can be found (see Fig. 2.3). In the diffusional deposition regime (very small particles with $\tau_p^+ < 0.2$) as $\tau_p^+$ increases the deposition rate decreases. In this regime particle transport is well represented by a gradient diffusion model, that has to account both for the turbulent diffusion (in the bulk flow) and Brownian diffusion in the region adjacent to the wall. In the diffusion-impaction regime ($0.2 < \tau_p^+ < 10^{-2}$) there is a dramatic increase of several orders of magnitude in the deposition rate as the particle time constant increases. This increase is mainly due to the interaction of particles that have significant inertia with turbulent fluid eddies, making it the most interesting regime in turbulent dispersion studies. In this regime, turbulent diffusion and inertia-dominated mechanisms together play an important role. In the third regime (known as inertia-moderated regime), particles having very high inertia acquire sufficient momentum from eddies in the turbulent core to reach the wall. Here diffusion plays a very small part
and deposition tend to decrease as the particle time constant increases as the response to the turbulence becomes weaker. Two sets of particles belonging to the diffusion-impaction regime has been chosen, that match all the criteria previously discussed and are in the range of response times considered in literature. The density ratio between the particle and the fluid has been set to 1000 (a common choice in similar works) to account both for water droplets in air and for particles made with substances with specific weight similar to water (e.g. polystyrene, commonly used in experiments).

The properties of the chosen particles are reported in Table 2.1. This set of particles is the same as those used by van Harleem et al. [59] for their simulations. Their work has been taken explicitly as a reference to validate our results since they performed Lagrangian particle tracking in conditions similar to those used in the current work (i.e. open channel flow at low Reynolds number).
2.2.5 Computational procedure

The dimensions of the domain used to track the particles are $L_x, L_y$ and $L_z$ in the streamwise, spanwise and normal direction, respectively. The orientation of the coordinate system for the particle phase is consistent with the one used for the flow on the gas side.

The origin of the frame of reference for the particles in the case of deformable interface requires a discussion. Since the Lagrangian particle tracking code accepts orthogonal grids only, it is necessary to track particles in the mapped space. Thus, the particles coordinates are in the $(\xi_1, \xi_2, \xi_3)$ and not in the $(x, y, z)$ frame. Since back-transforming the position of every single particle in the domain from mapped to physical space is computationally too expensive, it was decided to assume for the particle a reference adhering to the surface. In this way, particle positions in OCH and FDI case can be compared in a consistent way (in both cases, $z^+ = 0$ refers to the coordinate of a particle whose center is in contact with the surface). Moreover, since the waves have small amplitudes (‘capillary waves’), the differences between normal coordinates in the two reference frames are always small and can be neglected. Spanwise and streamwise positions don’t cause problems since the metrics are maintained between the two spaces in these directions.

The initial distribution of particle positions has been set homogeneous over the computational domain. The positions of the particles are chosen randomly and their initial velocity was set equal to the interpolated fluid velocity at their position.

When a particle leaves the domain across the outflow plane (at $x^+ = L_x$) or in the spanwise direction (at $y^+ = 0$ or $y^+ = L_y$) periodic boundary conditions are applied both for position and velocity of the particle.

The lower and upper boundaries are considered to be completely adsorbing, i.e., a particle at a distance less than one particle radius from these boundaries is removed.

Since the total number of particles has to remain constant in time in order to reach statistically stationary conditions, when a particle deposits at the lower or the upper boundary, it is removed, but another one is reintroduced in the domain at the inflow plane (at $x^+ = 0$). The spanwise and normal coordinates of the
re-introduced particle are chosen randomly and their velocity is set equal to the fluid velocity at that position. From a physical point of view this procedure is not strictly correct because the particle velocity is not equal to that of the fluid at the inflow plane. Thus, the velocities of the re-introduced particles are necessarily affected by the imposed initial conditions for a certain amount of time. According to the arguments presented by van Harleem et al. [59] the estimated distance covered by a St=15 particle in this adjustment time interval is approximatively ten times the height of the channel (approximatively 1710 wall units). Since this length is larger than the streamwise dimension of the computational domain ($l_x$, see Section 2.1), a longer domain has to be adopted to appropriately track the particles. The streamwise extension has been set to $5 \times l_x$, whereas spanwise and normal dimensions are kept unchanged ($l_y$ and $l_z$, respectively). The dimensions of the particle computational domain are thus $L_x = 5370$, $L_y = 537$, $L_z = 171$ wall units. The fluid velocity at every grid point was simply obtained by extending the original flow five times in the streamwise direction. Moreover, for most of the analysed quantities, only the particles that are located at more than 1710 wall units away from the inflow plane were taken into account. The fluid velocity at every grid point was simply obtained by extending the original flow five times in the streamwise direction.

The advantage of this procedure is twofold: firstly, statistical quantities can be computed as a function of the streamwise coordinate and secondly there is always a sufficient number of particles with a velocity independent of the imposed initial condition at the inflow plane.
2.3 Parametric study

In order to quantify the effects of the choice of the numerical parameters on the statistics obtained from the Lagrangian particle tracking, a parametric study has been conducted. This analysis has as been carried out only for the OCH case, and the results assumed valid also for the FDI case.

An entire set of small simulations have been performed and, for each of them, the cumulative number of particles that deposit at every non-dimensional time-interval has been calculated. Some preliminary tests show that this statistical quantity is very sensitive to the choice of parameters. In the neighborhood of the wall, in fact, where the processes that control the deposition occur, steep gradients in the velocity field are present. As a consequence, a careful choice of the interpolation scheme adopted to evaluate the fluid velocity at the particle position is very important in this region. Since the fluid velocity is very small at this location, the way the velocity and position of the particle is calculated at every time step (i.e. the integration method) could affect the deposition as well. As already mentioned, the rate of deposition increases according to the increase of particle inertia. The number of particles that deposit at every instant, as a consequence, is expected to be lower for the St=5 particles than for the St=15 ones. Moreover, the heavy particles, having greater inertia, are more likely to come from greater distance from the wall than the light ones, where the effect of the interpolation and integration scheme is weaker (since the gradients are smoother). Taking into account the previous observations, this tests consider only the deposition of St=5 particles on the flat wall and in the free-slip boundary (i.e. OCH case), in order to limit the number of test cases considered.

The number of particles used for the simulations has also been evaluated. As is obvious, the accuracy of every statistical quantity increases with the number of particles, but accordingly the computational effort in tracking the particles increases as well. The balance between the needed statistical accuracy and the computational resources employed leads to the final choice of the number of particles tracked.

The assumption on how the boundary conditions are implemented can be questioned if one thinks that in reality, as the particle approaches the wall,
Figure 2.4: Cumulative number of particles that deposit for different integration schemes; (a) lower boundary, (b) upper boundary.

it is subject to physical mechanisms that are not accounted for in this work (electrostatic attraction, coalescence with other droplets/particles etc.). As a consequence, a particle could be considered deposited when it is at distance from the wall greater than one particle radius (e.g. two or three particle radii). A numerical evaluation of the proper choice of the plane at which the particles can be considered deposited has also been performed.

2.3.1 The effect of the integration scheme

The integration schemes tested are second order Adams-Bashforth and second and fourth order Runge-Kutta methods. The simulations have been performed for 870 non-dimensional time units using 13056 particles and the fourth order interpolation scheme. Results for each boundary are shown in Figs. 2.4. At the wall the Adams-Bashforth method underpredicts the particle deposition compared to the Runge-Kutta method. For the latter scheme, no remarkable differences between the order of integration can be noticed. Moreover, from Fig. 2.4 (b), it can be argued that the choice of integration scheme does not affect the deposition at the free-surface. Therefore, the fourth order integration scheme was chosen for the simulation.
2.3.2 The effect of the interpolation scheme

The Lagrangian particle tracking code offers the choice between second, fourth and sixth order for the interpolation of the fluid velocity at the particle position. Figures 2.5 (a) and (b) compare the three methods. For this test, the fourth order, Runge-Kutta method for the integration of the particle velocity has been adopted and 13056 particles have been tracked. The sixth-order interpolation predicts a significantly higher deposition at the wall. The number of particles deposited is however too low to evaluate how relevant is the choice of an high order interpolation scheme for the purpose of calculating the steady-state deposition rate. Hence, two longer simulations (≈5000 non-dimensional time units) have been performed comparing the fourth and sixth order scheme. After approximately 3400 non-dimensional time units the number of particles predicted
by the fourth order scheme is higher than the one predicted by the sixth order one. As it can be argued from the figure, the two curves reach an almost equal asymptotic value at the end of the simulation. The calculated deposition rate at statistically stationary state, as a consequence, will not be significantly affected by the choice of interpolation scheme. As a consequence, the choice of the fourth order scheme is a good compromise between efficiency and accuracy.

The examination of the deposition at the free-slip boundary shows that the fourth order scheme is almost as accurate as the sixth order one. This result, together with the previous one regarding the effect of the integration scheme, suggest that deposition at the upper boundary is quite insensitive on the numerical parameters adopted, as expected being the gradients in the velocity field very smooth in the region near the free surface.

2.3.3 The effect of the number of particles

In Figures 2.7 the cumulative number of particles deposited at the wall, normalized by the total number of particles released in the domain, is shown. For this statistic, three test simulations have been performed using 10000, 50000 and 100000 particles, tracked adopting a fourth order Runge-Kutta method for integration and a fourth order accurate method for the interpolation. These simulations are performed for around 1800 non-dimensional time units. In particular for the deposition at the free-slip surface, the three plots are quite overlapping, suggesting that 10000 particles could be enough to study the deposition rate. On the other hand, following Young and Pope[65], the statistical sampling error decreases as $N_p^{0.5}$; as a consequence tracking 100000 particles can yield statistics that are three times more accurate than tracking 10000 particles. Test simulations suggest that tracking a larger number of particles (e.g. 300000) results in a great increment in the computational resources needed. This does not correspond, however, to a substantial increase in the statistical accuracy and in the quality of information that can be extracted from the simulations. As a consequence, 100000 particles are considered enough for the purposes of the present project.
2.3.4 The choice of the boundary condition for the particle phase

Figure 2.8 shows the cumulative number of particles deposited if three different planes, where deposition is assumed to occur, are chosen. These are located at one, two and three particle radii from the wall. A total number of 13056 particles are tracked in this case for approximatively 5400 non-dimensional time units, using the fourth order Runge-kutta method for the integration and the fourth-order interpolation scheme. The increase in the deposition for a slight change in the plane position is dramatic. A crude estimate of the deposition rate, based on the slope of the curve at the end of the simulation, has been compared to values found in literature. The calculated values overpredict the experimental deposition rates by orders of magnitude. This suggests that the assumption that particle deposit when it is at one particle radius of distance from the wall is correct from a physical point of view, or at least it is a satisfactory numerical description of reality.
2.4 Adopted numerical parameters

The final choice of numerical parameters for the simulations is a consequence of previous analysis and it is summarized in the following list:

- **Integration scheme**: Fourth order Runge-Kutta
- **Interpolation scheme**: Fourth order Lagrangian polynomials
- **Number of particles**: 100000

The boundary conditions are implemented as described in Section 2.2.5. The same volume fraction of particles has been used for both for both the FDI and the OCH case. Particles have been tracked for 5436 and 2355 non-dimensional time units in the OCH and in the FDI case, respectively. In fact, as it will be discussed in Section 4.2.2, a longer simulation was needed for the OCH case to obtain a statistically stationary condition. Data for the particles have been saved every 5 non-dimensional time units approximatively, for both the cases.
Chapter 3

STATISTICS FOR THE FLOW

Here the statistics for the continuous phase are reported. Only the statistical quantities that are useful in understanding the behaviour of the particle phase are presented, in particular the most suggestive for explaining the similarities and the differences between the flow over the deformable interface (FDI) and over a flat wall (OCH). As already mentioned in Section 2.1, the simulation of the turbulent flow is not the objective of this project. Thus, the reader is referred to the work of Fulgosi et al. [21] for detailed information.

3.1 Velocity field

3.1.1 Mean velocity profiles

Figure 3.1 shows the profiles of the mean streamwise velocity for the the FDI and OCH case. The velocity profiles are practically the same except that the interfacial velocity in the FDI case is not zero because of the applied boundary conditions.
3.1.2 RMS velocity profiles

The distribution of turbulence intensities is almost identical in the two cases, but again, because of different boundary conditions, the RMS values of $u$ and $v$ in the FDI case do not originate from the same location. The values of turbulence intensity, for the three components of velocity, are significantly higher near the deformable interface. With respect to the objectives of this work, the values of turbulence intensities in the vertical direction are shown for the region $z^+ = 0 - 5$, in Figure 3.2 (b). The RMS of $w$ is considerably enhanced by the presence of the deformable boundary. In particular, at the first grid point $z^+ = 0.1$ there is an increment of the intensities of almost 60 times, as shown in Fig.3.3 (a). The differences are sensible up to $z^+ \approx 3$. The correlation coefficient between the normal velocity fluctuation at the deformable interface and in the near surface region (Fig.3.3 (b)) has also been calculated. The flow field perceives the presence of the moving boundary up to an height of 5 wall units. 90% of the correlation is within 3 wall units. The data for the RMS velocity fluctuation have also been compared to those of van Harleem et al. [59]. This comparison showed significant differences, in particular for the normal and spanwise RMS, with values up to 15% lower than our data.
Figure 3.2: (a) RMS profiles of the three velocity components. Lines and symbols are used to identify FDI and OCH, respectively. (---) and (o), streamwise velocity; (-----) and □, spanwise component; (---) and (△), normal component, (b) RMS of vertical velocity fluctuations near the interface/wall.

Figure 3.3: (a) Ratio between normal turbulent intensities of the FDI and OCH case, (b) Correlation coefficient between the RMS of $w$ at the deformable interface and in the near surface region.
3.2 Flow structure

The near wall/interface region is characterized by active turbulent motions. Active motions make essential contribution to the shear stress, while inactive motions are simply random events (i.e. there is no correlation between streamwise and normal velocity fluctuation). A quadrant analysis has been conducted to quantify the contribution of the active events. These motions have been divided into four categories (Fig. 3.4): first quadrant events (I), characterized by outward motion of high-speed fluid; second quadrant events (II), characterized by outward motion of low-speed fluid (commonly referred to as *ejections*); third quadrant events (III), characterized by inward motion of low-speed fluid; and finally, fourth quadrant events (IV), characterized by inward motion of high-speed fluid towards the wall (the so-called *sweeps*). Sweeps and ejections are considered the major turbulent producing motions contributing to positive turbulent kinetic energy production.

A comparison of the fractional contribution of each type of event (Fig. 3.5) shows that ejections and sweeps act at the same locations as in channel flow with similar contribution. In the core flow first and third events are slightly enhanced for the FDI case. Fluid motions towards the wall/interface dominate within $z^+ = 12$ from the lower boundary.

The action of the the “quasi-streamwise” vortices (Banerjee et al. [3]) that populate the near wall region leads to the formation of the characteristic “streaky structure” of the velocity field. This consists in the alternation between regions where fluid velocity in the streamwise direction is lower than the mean (usually referred as *low-speed streaks*) and high-momentum fluid (i.e. *high-speed streaks*). These patterns are intimately related to the shear producing events (i.e. sweeps and ejections, mainly) trough a mechanism that, described in a simplistic way, is depicted in Fig.3.6.

To study the flow structure in relation to the streak formation, the non-dimensional shear rate parameter $\tilde{S}$ introduced by Lam & Banerjee [32] was employed. It is defined by

$$\tilde{S} = \frac{dU}{dz} \frac{|\tau_{wn}|}{\varepsilon} = \frac{\mathcal{P}}{\varepsilon}$$

and represents the ratio of the rate of production of turbulent kinetic energy
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Figure 3.4: Analysis of the shear contributing events in the $u - w$ plane.

Figure 3.5: Quadrant analysis terms. Lines and symbols are used to identify FDI and OCH, respectively. (---) and (+), first quadrant events; (—) and (+), second quadrant events; (····) and (△), third quadrant events; (−·−) and (◦), fourth quadrant events.

to its dissipation rate. If $\tilde{S} > 1$ the shear is high enough for streaks to form, indicating that mechanical generation of turbulence is still dominant over dissipation. From Fig.3.7 it can be seen that the formation of the streaks take place at the same distance from the interface/wall (roughly at $z^+ \approx 8$) but it seems that it penetrates deeper into the core flow. The difference, quite perceptible in the core flow where the streaks are no longer visible, mainly reflects the alternate and disaggregate way these structures form below $z^+ \approx 40$, as can be seen in Figure 3.8.

The streaky structure in the channel flow appears to be more regular than on top of the deformable interface; the clear alternation between high and low speed regions is also more visible, while the streaky pattern looks overall less organized. However, the streamwise elongation of the streaks does not seem to be affected by the interface deformation.
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![Diagram of Quasi-streamwise vortices with labels Ejection, Sweep, and Ejection indicating flow directions.]

Figure 3.6: Interaction between streamwise vorticity $\omega_x$ and streaky structure.

![Graph showing profiles of the non-dimensional shear-rate parameter with lines and symbols used to identify FDI and OCH, respectively.]

Figure 3.7: Profiles of the non-dimensional shear-rate parameter. Lines and symbols are used to identify FDI and OCH, respectively.

![3D views of streaky structure in (a) FDI and (b) OCH cases, with light blue and gold colors indicating low and high speed streaks respectively.]

Figure 3.8: Three-dimensional view of the streaky structure in (a) FDI and (b) OCH cases. Light blue and gold colors indicate low and high speed streaks respectively.
Chapter 3. STATISTICS FOR THE FLOW

3.3 Coherent structures identification and visualization

Hussain [24] defines a coherent structure as a connected, large-scale turbulent fluid mass with a phase-correlated vorticity throughout its spatial extent. Another definition of coherent structure, given by Robinson [49], is a “three-dimensional region of the flow over which at least one fundamental flow variable exhibits significant correlation with itself or with another over a range of space and/or time that is significantly larger than the smallest scales of the flow”. Non randomness, extension in space and duration in time thus seems to be the most important characteristics of this movements.

Three different identification criteria has been tested. These are:

- The so-called $Q$–factor proposed by Hunt [23], which is basically the second invariant of the velocity gradient tensor:
  \[
  Q = \frac{1}{2} (r_{ij}r_{ij} - s_{ij}s_{ij})
  \]  
  (3.2)

- The second largest eigenvalue ($\lambda_2$) of the tensor $s_{ik}s_{kj} + r_{ik}r_{kj}$, defined by Jeong et al. [25].

- The streamline rotation vector, proposed by Perry & Chong [43]. The definition of this identifier (not formally reported here) is based on the classification of complex flow fields by the identification of their three-dimensional critical points.

All the three different eduction techniques proved to provide the same level of detail in describing the flow structure. In Figure 3.9 two snapshots of isosurfaces of the streamline rotation vector has been shown in order to compare the FDI and OCH case. It appears that the vortical structures in the FDI case are more elongated and more streamwise oriented than in the OCH case. Moreover, the vortical field in the latter case appears more fragmented and irregular as compared to FDI. These impressions are confirmed by the inspection of several instantaneous pictures of the flow.

The effect of interfacial motion on the quasi-streamwise vortices has been analyzed in a statistical way by using the $-\lambda_2$ identifier. In Figure 3.10 the mean
and RMS profiles of the eigenvalue ($\lambda_2$) are reported as a function of the normal coordinate. In both FDI and OCH cases the mean values of $-\lambda_2$ is negative and comparable to its RMS value for $z^+ < 10$, reflecting that the viscous sublayer does not contain vortices. The peak RMS values occur within $10 < z^+ < 30$, suggesting the prominence of vortical structures in the buffer region. The free-slip surface is populated by coherent motions that are quite different from those found near the sheared boundary. In experimental investigations [45] and DNS [38] of wall bounded flows mainly three types of coherent structures have been identified. These are noted as upwellings, downdraft, and attached vortices. The upwellings are caused by the impingement of blobs of fluid originating directly from the wall onto the free-slip surface. On reaching the free-slip boundary these blobs spread out over the surface and form vortices at their edges. These vortices have their axis perpendicular to the surface, remaining attached to the surface for long periods of time. Finally, the interactions between upwellings near the surface may cause downdraft in which the fluid moves away from the surface. Figure 3.11 shows a contour plot of the normal velocity in the region
near the free-surface, for the flow over deformable interface. Hot colors refer to the upwellings, cold colors to the downdrafts. Attached vortices are marked with streamlines. The same structures of flow over a flat plane are characteristic also of the FDI case. This is clear also considering Fig. 3.12 (a) and (b), where instantaneous flow field parallel to the \( x - y \) plane at a distance of 6 wall units from the free-slip surface are shown in order to compare the OCH and the FDI case.

### 3.4 Summary

The overall picture that previous considerations suggest is that, from a quantitative point of view, the two flows are quite similar as regards turbulence properties. Comparison shows, in fact, a similarity in the distribution of turbulence intensities, suggesting that the lighter phase perceives the interface like a flexible solid surface. The major differences are localized in the region immediately adjacent to the wall/interface, as expected. The same coherent structures (i.e. streaks, sweep, ejections, vortical structures) populate the flow, although slight differences in the topology of these characteristic fluid motions have been noticed.
Figure 3.11: Contour plot of free-surface coherent structures.

Figure 3.12: Vector plot of the velocity field in the $x - y$ plane located at $z^+ = 165$; (a) OCH, (b) FDI.
Chapter 4

ANALYSIS OF PARTICLE DISPERSION

4.1 Numerical considerations about the DNS of particle dispersion

This section presents some general issues related to the way the statistics have been obtained and observations that can be useful in understanding the subsequent discussions. This considerations stress the importance of a correct working methodology: extracting data from the simulations that are physically meaningful is as important as correctly interpreting the data themselves.

4.1.1 Effect of initial conditions

In all our simulations, particles are released in the domain with a initial velocity equal to that of the fluid at the particle position. The initial mixing of the dispersed phase is mainly due to the entrainment caused by the flow rather then to the fluid-particle interaction. Every modification to the initial distribution is purely artificial at the beginning of the simulation and is therefore very important not to consider it as a part of the natural evolution of the Probability Distribution Function (PDF) of the particle position.

The time needed by the particle phase to loose the influence of the initial
velocity and redistribute into the flow, can roughly be estimated to be 760 non-dimensional time units at least, double the time known as *flow throughput time*. This is the time that a particle, convected with the velocity of the mean flow ($\overline{U}^+ \approx 14$), takes to traverse the whole domain length. This has been evaluated in the present simulations as:

$$t^+ = \frac{L^+}{\overline{U}^+} \approx 380$$

In the current work, every statistical quantity has been determined after at least 760 non-dimensional time units from the beginning of the simulation.

Although the value of 760 time units is only indicative, this basic analysis shows that in a small simulation (e.g. 1000 non dimensional units), most of the data obtained might probably be affected by the initial particle velocity. This concept is explained in the context of Fig. 4.1, where the time evolution of the normal velocity at deposition at the lower boundary, instantaneously averaged over the particles attaining one particle radius from the wall/interface is presented. As it can be seen, within 100 non-dimensional time units from the beginning of the simulation, the reported velocity is unnaturally high, with values typical of the bulk fluid velocity.

Note also that that the conditions at the inflow plane affect the particle statistics. In Section 2.2.5 it has been pointed out that particles must travel at least 1710 wall units before their velocities can be considered independent from
Chapter 4. ANALYSIS OF PARTICLE DISPERSION

initial conditions, imposed when they are reintroduced into the domain. In this respect, the data of the particles present in the first 30% of the domain length are simply not reliable. Most of the statistics for particle velocities and spatial distribution, are hence taken in the center of the computational domain or at its end. The effect of the inflow plane on particle distribution is better explained when considering the statistics in the streamwise direction: the behaviour of the dispersed phase at the beginning of the channel (where the particle are reintroduced) is considerably different from the one in the rest of the domain.

4.1.2 The effect of extending the flow periodically

The procedure of extending the domain in streamwise direction (Section 2.2.5) has a natural shortcoming: instantaneously, the same flow patterns are periodically repeated every 1074 wall units. The distribution of the particles in the bulk flow remains quasi-uniform in time and moreover is roughly independent of the streamwise position. The expected result is that some repeating pattern in particle distribution will instantaneously form in the flow, since the same flow structures act periodically on the particles. Averaging in time therefore should remedy this instantaneous effect. But instead, it has been found that the time-averaging interval adopted is not enough to obtain statistics independent of the flow periodicity.

In fact, repeating particle patterns form also inside the viscous sub-layer, without loosing spatial coherence during most of the simulation. At these distances from the lower boundary there is no much mixing, in particular for the OCH case, since turbulent fluctuations are weak and streamwise velocity is almost negligible. Fig. 4.2 shows instantaneous particle distribution in the OCH case in the zone \( z^+ < 5 \) for the St=5 particles. The two snapshots have been taken at two time intervals, distant 880 non-dimensional time units (almost 20% of the simulation). It is clearly recognizable that similar particle distribution patterns in this region repeat three times in the streamwise direction. Moreover, strong similarities in the distributions can be noticed also between the two snapshots, in spite of the fact that the time interval between the two is considerable. These similarities suggest that in the region where this massive particle patterns form, the time scales characterizing the changes in particle distribu-
4.1.3 Statistical steadiness

A particle dispersion scenario can be considered statistically stationary if every statistics is independent of time. This criterion is not absolute (i.e. every single statistical quantity takes different time to reach a stationary condition) which implies the necessity to conduct for each statistics, a preliminary analysis to determine the most suitable instant to start averaging and for how long it should be performed. It has been found that the statistic that takes a longer time to be time independent is the wall normal concentration profile; the others are
essentially dependent on this latter one (e.g. the number of particles deposited in time and thus the deposition rates).

4.1.4 Slab size for space averaging

The particle concentration in dilute suspensions is far from constituting a continuous field. Furthermore, as the simulation proceeds, the distribution of the dispersed phase become nonhomogeneous. In fact, it features zones of strong gradients (in particular in the normal direction), zones where hardly a particle is present, and also zones in which the volume fraction of the dispersed phase is very high. The definition of the measuring volume used to calculate the particle concentration (hereinafter referred to as slab size or bin size) is thus a non-trivial problem. In fact, the spatial scales characterizing changes in the particle field are comparable to the size of the bin. To make the concept clear, let us suppose that all the particles are residing in the region $0 < z^+ < 1$ (and this assumption is not far from reality, as we shall demonstrate in Section 4.2.2). If the concentration is calculated by use of two different slabs, one with a height of two wall units and the other of one wall unit, the concentration in the first case will clearly be half with respect to the second one. This problem clearly arises when one tries to compare data between the previous works; in particular for the normal concentration profile calculated in similar conditions (i.e. same Reynolds number and choice of particle parameters) there is a profound disagreement between different authors (e.g. [29, 48]). The only way to be granted that the measurement can be repeated is to exactly specify the slab size used, maintaining it small enough to capture in detail the particle distribution gradients.
4.2 Particle concentration statistics

4.2.1 Streamwise concentration profiles

Figure 4.3 compares the development of the streamwise concentration profiles. The statistics were obtained by dividing the entire domain length in cross stream bins of 200 wall units each. The mean volume concentration in every bin was normalized with the concentration in the case of uniform particle distribution over the entire domain. The appearance of a concentration gradient in the particle distribution is determined by examining the balance between the outward flux due to deposition and the net inward flux due to the particles coming from the upstream slab (which is obviously higher in the first slabs).

As expected, the mean slope of the line indicating the mean concentration is monotonically decreasing, everywhere except in the very beginning of the domain length (approximately from 0 to 1000 wall units). It is not useful to analyze this location, since this is the region of the domain where velocities of the particles are still affected by the initial conditions at the inflow plane. Out of this region, the differences between the cases are not substantial: the slope of the curve is a bit higher for St=15 than for St=5, as expected since the deposition rate is higher for the first case (as we shall see in Section 4.3). However, the length of the domain is not extended enough to make this difference really evident. Instead it seems that the particle distribution is strongly affected by the periodicity of the flow in the FDI case, causing some repeating features which are also visible in the curve.

Figure 4.4 (a) and (b) show the streamwise concentration profile, obtained with the procedure described previously, accounting only for particles located in the region $3 < z^+ < 171$. The profile is straight, almost linear in this case, confirming the observation made in Section 4.1.2, that is: the periodic features are mainly due to particle accumulation patterns in the region adjacent to the lower boundary ($z^+ < 3$).
Figure 4.3: Streamwise development of particle concentration; (a) St=5, (b) St=15.

Figure 4.4: Streamwise development of particle concentration without considering particles residing close to the lower boundary; (a), OCH (b), FDI.
4.2.2 Normal concentration profiles

Figures 4.5 and 4.6 depict the time evolution of the normal concentration profiles, i.e. the instantaneous number of particles present in bins parallel to the lower boundary, divided by the volume of the bin and normalized by the value of concentration for uniform distribution.

Since this statistic serves only for a qualitative description, the concentration profile has been obtained by performing space average over the entire domain length and width. This is obviously not a strictly correct procedure because of the non negligible concentration gradient in the streamwise direction. Here, the height of the slabs in the normal direction changes according to the normal grid spacing (i.e. it is not constant). Instantaneous profiles at the beginning of the simulation and after the stationary state was achieved, have been arbitrarily chosen to show the temporal evolution of the phenomenon. There is a strong tendency of the particles to migrate towards the lower boundary, and this migration seems to be faster for the high Stokes particles.

The normal concentration distribution is due to the instantaneous balance between fluxes due to two main contributions: ‘turbulent diffusion’ acting to smooth concentration gradients and is well defined even in the case of homogeneous turbulence, and ‘turbophoresis’, effect recognized independently by Camparaloni [8] and Reeks [47], that is: in inhomogeneous flows, particles migrate from regions of high to low turbulence intensity. The time evolution of the normal concentration profile indicates clearly that turbophoresis plays an important role in dispersion. Since the initial particle distribution is homogeneous and the initial velocities of the particle are randomly distributed as the velocity of the fluid, there is an equal probability of the particle to move towards the lower boundary and away from it. There is no other way to achieve so quickly an asymmetric distribution if we suppose that dispersed phase evolve just because a law of diffusion similar to Fick’s law. In this case, in fact, an initially homogeneous particle distribution would remain homogeneous for long times.

The overall shape of the calculated profiles is mainly controlled by particle accumulation very close to the lower boundary. In fact the concentration in the bulk flow is very low and is only slightly time dependent.
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Figure 4.5: Time evolution of the normal particle concentration profile for the OCH case; (a) St=5, (b) St=15.

Figure 4.6: Time evolution of normal particle concentration profile for the FDI case; (a) St=5, (b) St=15.
Figure 4.7: (a) Time series of concentration in 2 slabs very close to the wall, (b) Time series of the number of particles near the wall as a function of time.

Figure 4.7 (a) shows a time series of particle concentration in two slabs adjacent to the wall ($0 < z^+ < 2.67$ and $2.67 < z^+ < 5.84$) for St=5 and OCH case. The concentration at the wall is continuously growing with time and reaches a quasi-constant magnitude only after 4500 time units. The concentration value in the second slab is instead decreasing. The particles are thus transported to the wall where they accumulate, spending there a long time before finally depositing. Although this is shown only for the lighter particles, this behaviour is characteristic of both sets of particles in the wall-flow simulation. In FDI case, however, the deposition mechanisms are more efficient and the particles spend less time in the near interface region before deposition. This is clearly evident in Figure 4.7 (b), where the time series of the number of particles present in a slab adjacent to the lower boundary ($0 < z^+ < 2.67$) is presented, comparing OCH and FDI cases. While in FDI this number starts oscillating around an almost constant value only after 1000 time units, it is continuously growing in OCH, in particular for the St=5 particles, indicating that no steady-state condition is reached in the particle normal distribution.

Particle concentration profiles at equilibrium (i.e. when convergence is achieved) are shown in Figure 4.8. In this case, the bin vertical extension dimension has been kept constant ($\Delta z^+ = 0.15$). The distribution refers to a region located in the center zone of the computational domain ($x^+ = 2400–2600$), and it has been obtained by normalizing the time-averaged concentration in every normal slab to the average concentration of particles in the region considered (i.e. setting the integral across the channel height and width equal to unity).
The differences between concentration values at the wall/interface shown in Figure 4.8 and in the plots referring to the temporal evolution of the particle normal distribution are evident: this is due partly on the more refined bin size (see Section 4.1.4) and partly due to the fact that the previous ones were only instantaneous profiles. A large increase in particle concentration very close to the interface/wall is observed, in particular in OCH configuration. The peak value is located around $z^+ = 1$ in FDI and $z^+ = 0.3 - 0.4$ in OCH. The particles accumulation in the wall bounded case is higher for St=5 particles than for St=15 particles.

Particles accumulation near the wall has also been observed by other authors (e.g. [37, 44, 59, 60]) in both numerical simulations and experiments; it has been even considered as a severe test for model validation ([48]). However, as pointed out in Section 4.1.4, there is a lot of disagreement between the values and the way the statistics are obtained. In particular Van Haarlem and co-workers [59], who performed a Lagrangian particle tracking in conditions similar to those considered in the present work and with the same set of particles, do not report so high peaks near the wall (their values at the lower boundary are in the order of 10). This is probably due to the bigger bin size they have used. In fact, since their first bin size was ten times bigger then the one used in the present study, they probably could not catch the phenomena characterizing particle distribution at distance from the wall less then 1 wall unit. In van Harlem’s work, as well as in various others, accumulation of particles at the lower boundary is reported to be higher for the high Stokes number particles. This trend is confirmed for the OCH case, but only up to a distance of $z^+ \approx 0.4$. Very close to the wall, however, the trend is inverted. In this region, the phenomenon of accumulation is dominated by the deposition flux and not by the mechanism of segregation that leads the particles towards the wall.

In the FDI case, the concentration for the lighter particles is higher everywhere and the actual values of concentration are approximatively an order of magnitude lower than in OCH case. Moreover, the distribution is smoother and the gradients are less sharp. This is probably due to the mixing effect that the non-negligible fluid fluctuations near the interface have on the dispersed phase.

It is interesting to note that there is also a slight accumulation of particles
in the upper boundary for all the cases considered, with values 2 to 3 times larger than the bulk concentration. This phenomenon has also been observed by van Harleem [59]. If turbophoresis acts in dragging particles of high-to-low turbulent intensity, this behaviour can then be well explained. In fact, fluid turbulence intensity in the normal direction decreases approaching the free-slip surface.

The concentration in the bulk flow is in the order of the one obtained in case of uniform concentration. Figure 4.3, in fact, suggests that the value of concentration in the region \( x^+ = 2400 - 2600 \) is very close to the value \( C_u \), and this is trivially the integral across domain cross section that is used as a reference quantity for the profile at equilibrium.

It has already been shown in Section 4.2.1 that the mean concentration decreases in streamwise direction because of deposition. In other words, \( \langle C(z) \rangle \) is also a function of \( x \). As pointed out by Young & Leeming [66], the normal particle distribution is self similar if it is scaled with the mean concentration at the location where the distribution is evaluated, i.e.:

\[
\langle C^+ \rangle = \frac{\langle C \rangle (z,x)}{C_m(x)} = \langle C^+(z) \rangle
\]

Figure 4.9 (a) and (b) show the concentration distribution at different stream-wise positions for the OCH and the FDI configurations respectively, normalized by reference to the scaling proposed by Young & Leeming. The profiles, which
4.3 Statistical analysis of particle deposition rates

The deposition at the boundaries is a time-dependent phenomenon for a large part of the simulation duration. This is shown in Fig.4.10, reporting the cumulative number of particles that hit the boundaries as a function of the non-dimensional time. Examining the OCH case, reveals the slope of the curve to reach an asymptotic value towards the end of the simulation. This reflects the fact that after a transient period in which particles redistribute themselves into the domain, the number of particles deposited every instant of time is almost constant, as compared to the time scale characterizing the variations in the particle distribution. The deposition is dependent on particle inertia, being larger for $St=15$ than for $St=5$ on both boundaries. Considering the wall bounded flow, the deposition of the lighter particles on the lower boundary is remarkably low; significant values can be observed only at the end of the simulation. The underlying process is that a large number of particles with this low inertia resides very close to the wall and keep continuously accumulating. Particles neither deposit for long times nor are significantly re-entrained in the core flow.
Figure 4.10: Cumulative number of particles deposited at either boundaries; (a) OCH, (b) FDI.

once reaching the near wall region. This phenomenon was observed by Brooke et al. [5] and by Kaftori et al. [27], and it characterizes mainly experiments with small particles and low shear rate.

The number of both St=5 and St=15 particles deposited on the upper boundary is always larger than that at the lower boundary. On the other hand, at the end of the simulation the curves referring to the two types of boundaries are almost parallel, i.e. the slopes of the curves reach an almost equal asymptotic value. Just as an estimate, this indicates that the steady state deposition rate is in the same order of magnitude for either boundaries.

The analysis of the results in the FDI case reveals remarkable differences: the deposition of St=5 particles in the lower boundary is significantly increased, reaching values comparable to those for the St=15 particles. On the contrary, bigger particles don’t seem to strongly feel the effect of the freely deformable interface, with their deposition rates being of the same order of magnitude in both FDI and OCH cases. Focusing on the differences between the two flows, the deposition on the upper boundary in FDI seems to follow different mechanisms than at the free-slip surface in the wall bounded flow, even if the cumulative number of particles deposited is of comparable level. In particular, the “bumps” in the curve in Fig.4.10 (b) suggest that the number of particles hitting the upper boundary in the flow over the deformable interface is intermittent, almost periodical. This effect is better represented in figure 4.11 where the instantaneous number of St=5 particles reaching the free surface is shown. The figure shows time intervals in which a large number of particles deposit, followed by
Chapter 4. ANALYSIS OF PARTICLE DISPERSION

Figure 4.11: Number of particles depositing in the upper boundary for St=15.

periods when only a few particles collect. The non-dimensional deposition coefficient is presented in Fig. 4.12 as a function of the streamwise coordinate. Here slabs of $\Delta x^+ = 200$ are used. However, the tests performed showed that the calculated quantities needed for these statistics are quite insensitive to the exact value of the slab length.

The deposition coefficient is the mass transfer coefficient of the dispersed phase at the boundary, calculated based on the assumption that on average, the number flux of particles that settle at the wall is proportional to the concentration of particle in the bulk flow:

$$K_d^+ = \frac{J_w}{C_m u_*}$$ (4.3)

where, $J_w$ is the mass or number of particles reaching the considered surface per unit area per unit time, $C_m$ is the mean bulk concentration of particles and $u_*$ is the friction velocity. Note that the concentration can alternatively be expressed in terms of number or mass density, as the suspension is mono-disperse (i.e. in a simulation, all the particles have same diameter and density).

Figure 4.12 shows the deposition rate to be quite constant along the streamwise direction in the OCH case, while in FDI is decreasing slightly, featuring strong oscillations. This reflect the fact that the bulk concentration and the deposition at the deformable interface are less correlated, or, at least in an average sense, their relationship is not as linear as in the OCH case. As a consequence, there could be high deposition in regions of relatively low number of particles evolving near the interface and vice-versa. Another interesting quan-
Chapter 4. ANALYSIS OF PARTICLE DISPERSION

The quantity to analyze is the average location where the particle tend to deposit along the streamwise direction. In this respect the deposition rate is not a suggestive statistic, since it includes the contribution of the bulk concentration. Figure 4.13 shows the cumulative number of St=5 particles depositing at every streamwise location (the slab length used is 200 wall units). It is clear that the main reason for the irregular profile of the line indicating the deposition coefficient in Fig. 4.12 is that particles collect in preferential zones also in the streamwise direction. This fact is more evident in FDI than in OCH, only because of image scaling. Moreover, the deposition decreases at the end of the domain length in the FDI configuration while it remains quite constant in the streamwise direction in the other one.

The calculated deposition rates on the wall for OCH case are reported in Table 4.3 compared to the values found in the literature. The values of the present OCH simulations are in general significantly smaller than those found in the reported experimental works: the comparison with the work of Liu & Agarwal [33] shows for instance the deposition to be three times lower; they are 40% to 60% lower than those of McCoy et al. [36]. Actually, it can be argued from Figure 2.3 in Section 2.2.4 that there is no consensus agreement between authors on the exact values of the deposition rate. In fact, experiments report a wide range of different deposition rate values for a given particle response time.

However, the general assumptions of the present simulations can be questioned at this stage. The inclusion of the Saffmann lift force on the particle equation of motion could enhance deposition as discussed in Section 2.2.3.

Figure 4.12: Deposition coefficient; (a) OCH, (b) FDI
Moreover, the near wall accumulation of particles being very high, other effects, not easily reproducible through a numerical simulation, could have became important (e.g. adhesion due to different physical mechanisms, surface roughness etc.). Turbulence properties can play an important role in explaining the disagreement, too. In fact, experimental databases are obtained in physical situation significantly different from those simulated here (e.g. pipe flow at higher Reynolds number).

<table>
<thead>
<tr>
<th>EXP/DNS</th>
<th>St=5</th>
<th>St=15</th>
</tr>
</thead>
<tbody>
<tr>
<td>McCoy (exp.,[36])</td>
<td>0.0081</td>
<td>0.073</td>
</tr>
<tr>
<td>Liu &amp; Agarwal (exp.,[33])</td>
<td>0.015</td>
<td>0.135</td>
</tr>
<tr>
<td>van Harleem et al. (DNS,[59])</td>
<td>0.0064</td>
<td>0.051</td>
</tr>
<tr>
<td>Current work (DNS)</td>
<td>0.0056</td>
<td>0.045</td>
</tr>
</tbody>
</table>

Table 4.1: Deposition coefficients from the current simulation (OCH case) and from previous works for the deposition at the wall.

The comparison with the work of van Harleem is instead very satisfactory. The small differences are easily explained considering the non-negligible differences in turbulence intensities between our flow field and the one used by these authors. The values obtained about the deposition at the free-slip surface have also been compared to those obtained by van Harleem et al. . The results are reported in Table 4.2.

<table>
<thead>
<tr>
<th>DNS</th>
<th>St=5</th>
<th>St=15</th>
</tr>
</thead>
<tbody>
<tr>
<td>van Harleem (DNS)</td>
<td>0.013</td>
<td>0.043</td>
</tr>
<tr>
<td>Current work (DNS)</td>
<td>0.008</td>
<td>0.047</td>
</tr>
</tbody>
</table>

Table 4.2: Deposition coefficients for the deposition at the upper boundary (OCH case)

Disagreement between the results are only slight, accounting for the differences between the two flow fields. Since the working procedure adopted by van Harleem has been quite closely followed, the satisfactory comparison with these author makes our simulation sufficiently validated. The comparison of Table 4.3 and Table 4.2 shows that the deposition values at the lower bound-
ary and at the upper boundary are very similar. The rough estimate made considering the cumulative number of particle deposited is therefore confirmed.
For the case in which the surface is free to deform, the computed values of deposition rate on the interface are reported in Table 4.3.

<table>
<thead>
<tr>
<th></th>
<th>DNS</th>
<th>St=5</th>
<th>St=15</th>
</tr>
</thead>
<tbody>
<tr>
<td>FDI case</td>
<td>0.052</td>
<td>0.071</td>
<td></td>
</tr>
</tbody>
</table>

Table 4.3: Deposition coefficients for the deposition at the deformable interface (FDI case)

The deposition rate is enhanced on the moving interface compared to that over the flat wall. The deposition coefficient is increased by about 9 times for St=5 particles and by 58% for St=15 particles. Further discussions (Section 4.8) are needed to correctly interpret these results, though it is already clear that the deposition on the freely deformable interface is not as sensitive to particle inertia as the deposition on the flat wall.

Values of the deposition rate in the upper boundary for FDI case are not reported here. In fact, as shown before, there the deposition is intermittent and not constant in time, thus the information given by a constant rate of particle collection at this surface may somehow be misleading.
4.4 Particle phase velocity statistics

Particles having finite inertia don’t follow exactly the fluid motions. Moreover, they are preferentially concentrated, both in the bulk flow and in the more active region near the solid boundary. For this reason the velocity distribution of the particle phase is not the same as the one of the fluid. Analyzing the first (mean) and second moment (RMS) of the velocity distribution for particle phase is the simplest and most suggestive way to examine this difference.

4.4.1 Mean velocity profiles

Figure 4.14 shows the mean streamwise particle velocity profile, compared to that of the fluid. Note that, since the profiles for the continuous phase are perfectly overlapping in OCH and FDI cases, at least in this image scale, the plot reports a generic “fluid” profile. Particles are on average slower than the fluid. This is quite surprising, if one considers the particles to have enough time to reach a velocity equilibrium with the main fluid stream. However this is consistent with previous results (e.g. Kaftori et al. [26]) and has been often brought as evidence of preferential concentration of particles.

No differences in the particle mean velocity between the OCH and the FDI cases can be observed, as shown in Fig.4.14. On the other hand, St=15 particles exhibit a slightly larger mean velocity than the St=5 particles, especially in the region $10 < z^+ < 15$. This behaviour has not been noticed in the work of
van Harleem et al. [59]. Actually, in their work, no differences has been found between the two sets of particles, even if this trend is consistent with results obtained in other previous numerical simulations ([50],[60]), where particles with larger Stokes numbers were employed (i.e. the heavy particles have an higher mean velocity than the light ones).

It is interesting to note that two experimental works (namely, Rashidi et al. [44] and Kaftori et al. [26]), report opposite trends for particles larger in diameter but with a smaller response time than those considered in our work. In particular, Kaftori et al. explained the trend describing the behaviour of particles coming from the near wall region and being retrained into the core flow. Since these particles have resided in a quasi-quiescent environment, they give negative contribution to the particle streamwise velocity in the bulk flow. Actually, the differences in Reynolds number for the flow and particle dimension between these works and current DNS are significant, so a direct comparison is difficult to achieve. Moreover the effect of gravity, that affect particles behaviour in the experiments, is not accounted for in the current work. However, some qualitative discussions can be made.

One explanation of the disagreement between the trends observed is that no significant retrainment of particles in the bulk flow has been observed in our simulation. This means that, once a particle reaches the viscous sublayer, it is hardly dragged back in regions of higher streamwise velocity, while this phenomenon (that is dependent on particle dimension and shear rate) is more common in experiments, also in the presence of gravity.

Another explanation to this phenomenon could be that it is dependent on the range of particle response time. Several works, mostly conducted in homogeneous isotropic turbulence (see, for a review, Eaton & Fessler [15]), show that there is a range of response times where strong preferential accumulation occurs, and this affects every statistics that compare fluid and particle phase velocities. Different trends considering different sets of particles could therefore be a consequence of this phenomenon.

Figure 4.15 shows the mean streamwise velocity profile obtained taking the fluid velocity at particle position rather then the particle velocity itself (essentially fluid particles instead of discrete particles). If the dispersed phase were
uniformly distributed over the whole domain (i.e. no preferential concentration occurs), the profiles for the fluid and for the fluid particles would coincide. The fact that this doesn’t happen in the same region where the largest deviation between the particle streamwise velocity and the fluid velocity occurs, suggest that particles are preferentially concentrated in this region of the flow. This observation reinforces the hypothesis that preferential concentration is the main cause of the observed trend in particle mean streamwise velocity. Even if the fluid has zero mean velocity in the vertical direction, on average the particles do have non zero normal velocity, as clearly shown in Fig. 4.16. This is consistent with the fact that particles deposit because there must be a mean drift flux of particles towards the boundaries for deposition to occur. The maximum negative velocity is located at \( z^+ = 20 - 25 \). This velocity, for \( St=15 \) particles, has an approximate value of \( \overline{W_p} \approx 0.15 \), while its value, for \( St=5 \) particles, is \( \overline{W_p} \approx 0.1 \). Quantitatively, similar results has been found by Young & Leeming [66] in pipe flow. This significant flux of particles is determined by balance between strong and coherent motions of fluid towards and away from the rigid boundary (probably these are the same sweeps and ejections events that control turbulence production,[34]). If the fluid motion is coherent in time, high Stokes number particles are transported towards the wall in the same way as the low Stokes number particles, but because of their inertia, high Stokes number particles could achieve greater velocities. The probability to reach the viscous sublayer and deposit is therefore higher. The population of particles in the zone \( 10 < z^+ < 15 \) is formed by particles residing in this region for relatively long

Figure 4.15: Mean streamwise velocity for the fluid at the particle position.
times (long enough to reach velocity equilibrium with the surrounding fluid) and particles coming from the core flow. These latter retain memory of the velocity achieved in those zones, influencing the streamwise mean velocity at the location where they pass. This phenomenon, together with preferential concentration, helps understand the reason why the mean particle streamwise velocity don’t coincide with the mean fluid streamwise velocity.

Looking again at Fig. 4.16, the symmetry of the profile is remarkable (zero mean value at $z \approx h^+$ and the same values close to the boundaries) in spite of the differences in turbulence characteristics near the two boundaries. This is reflected also in the fact that the values of deposition rate at the free-slip surface and at the rigid boundary are very similar for both sets of particles.

### 4.4.2 RMS velocity profiles

Turbulence intensity profiles in the normal, streamwise and spanwise directions are shown in Figs. 4.18, 4.19, and 4.17, respectively. As it can be observed, the particles do not follow exactly the fluctuations of the fluid in each direction. Since the strongest gradients in the particle concentration field are in the vertical direction, particle dispersion in turbulent boundary layer can be considered as a quasi two-dimensional phenomenon. In this respect, from a modeling point of
view, the RMS of particle velocity fluctuations in the normal direction, shown in Fig. 4.17, plays the most important role. From the figure it follows that there is no remarkable differences between the OCH and the FDI cases. Particles in the FDI case seems to follow fluid motions better then in the OCH case, although the differences are very slight. Light particles follow more closely the fluid in both OCH and FDI, confirming a well established trend. Only small differences can be noticed between St=5 and St=15. In other works, however, the differences were found larger than in the present work; even thought a direct comparison is difficult to achieve. In Table 4.4 some data found in literature are reported for comparison. From each reference, the maximum values of the RMS of normal velocity fluctuations for the fluid, the particle phase and the difference between the two, is reported. The comparison with the work of van Harleem et al. is not satisfactory. However, the fact that these authors report an RMS value for St=5 particles higher than the fluid raises some doubts on their averaging procedure. The comparison with Brooke et al. is satisfactory only for St=15 particles. For the other set of particles the lag between the fluid and the particles RMS should be smaller.

The fact that a stronger preferential concentration of St=5 particles occurs in the bulk flow could therefore be a possible explanation. Eaton & Fessler [18] showed that in the center of a closed channel, particles tend to avoid regions of high vorticity and low strain, a mechanism, that causes a deviation from a uniform distribution. This was found stronger for non dimensional response time approximatively equal to 5 (based on friction velocity and kinematic viscosity). In spite of the difficulties in comparing same Stokes numbers in different flows, (see [42]), their suggestion was that light particles are better concentrated than heavier ones.

<table>
<thead>
<tr>
<th>Author</th>
<th>Fluid</th>
<th>St = 5</th>
<th>Δ</th>
<th>St = 15</th>
<th>Δ</th>
</tr>
</thead>
<tbody>
<tr>
<td>Brooke et al. [6]</td>
<td>0.85</td>
<td>0.65</td>
<td>0.2</td>
<td>&lt; 0.55</td>
<td>&gt; 0.3</td>
</tr>
<tr>
<td>van Harleem et al. [59]</td>
<td>0.75</td>
<td>0.8</td>
<td>-0.05</td>
<td>0.65</td>
<td>0.1</td>
</tr>
<tr>
<td>Present DNS</td>
<td>0.82</td>
<td>0.5</td>
<td>0.32</td>
<td>0.45</td>
<td>0.35</td>
</tr>
</tbody>
</table>

Table 4.4: Comparison between indicative values of the RMS of particle and fluid velocity found in literature. Δ is the difference between the maximum RMS for the fluid and for the particle.
Figure 4.20 shows the RMS values of the fluid normal velocity fluctuations at particle positions, compared with the corresponding Eulerian statistics for the RMS of the fluid (i.e. obtained by spatially averaging over the whole domain). Lagrangian and Eulerian statistics for the flow differ more for fluid particles corresponding to St=5 than those corresponding to St=15; the lag is moreover larger for FDI case than for OCH case. Thus, St=5 particles are more preferentially concentrated, confirming the observations of Eaton & Fessler [18]. If this segregation occurs in zones with smaller velocity fluctuation than the mean, the observed large lag between the fluid and the particle RMS can be better explained. It is worth noting that the mechanisms of preferential concentration are somehow dependent on the volume fraction of particles used in the simulation. In fact, if in a simulation a very large number of particles is used in a simulation, the particle distribution is necessarily more homogeneous and the Lagrangian statistics are more close to their Eulerian counterparts.
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Figure 4.18: Turbulence intensity in the streamwise direction.

Figure 4.19: Turbulence intensity in the spanwise direction.
Figure 4.20: Fluid turbulence intensity at the particle position (normal direction).

4.4.3 Velocity distribution of deposited particles

The set of particles that deposit is only a small part of the population residing near the boundaries. In fact, each particle must satisfy two simultaneous conditions to deposit: (i) it has to be sufficiently close to the wall, and (ii) it should have high enough vertical velocity.

These two criteria are somewhat ambiguous and arbitrary, because they depend on particle inertia and, moreover, do not constitute two independent conditions. In fact, a particle could also come from regions not very close to the boundary but with high velocity, or from a region immediately adjacent to it but with a very small velocity. Moreover, the velocity acquired and the distance traveled are functions of the time during which the particle interact with the turbulent fluid motion (i.e. these variables are functions of the Stokes number).

Only a few studies have addressed this subject. The most quoted one is the work of Brooke et al. [6], who found that most of the particles that deposit have a relative high velocity, higher than the RMS value of velocity near the wall. This led them to conclude that the deposition occurs because of the 'free-flight' mechanism of deposition, pioneered by Friedlander and Johnstone [20]. This mechanism assumes that particles in the core flow are engaged in turbulent motions until they arrive at some not so well defined free-flight distance from the boundary. At this point they execute a flight towards the wall in a quiescent
environment (corresponding approximatively to the viscous sublayer). Since the fluid is relatively stationary in this region, the position \( z^*_s \) at which particles start free flying is related to the stopping distance of a particle thrown in fluid at rest, that is linked to particle inertia \( \tau^+_p \) by the relation [6]:

\[
z^*_s = \frac{V_{ff}^+ \tau^+_p}{K}
\]

(4.4)

the coefficient \( K \) accounts for the fact that the fluid is actually not exactly motionless in that region, and there is also some non-trivial fluid-particle interaction within a stopping distance from the wall. However, as pointed out correctly by Brooke et al., the coefficient \( K \) should be a weak function of particle inertia and of the order of unity.

The specification of the free-flight velocity \( (V_{ff}^+) \) is the main problem of this theory. While trying to match experimental data, several authors proposed to relate this quantity to the RMS of the fluid in the bulk flow, with some success but without improving knowledge about the mechanism ([52],[13],[4]).

In present work, the typical velocity of depositing particles has been statistically analyzed. Figure 4.21 shows the Cumulative Distribution Function (CDF) of the vertical velocities of the deposited particles. Here \( W_p \) is the velocity of the particle oriented towards the lower boundary. Read from right to left, it reports the probability that a particle deposit with a velocity higher than the value in abscissa. It is evident that particles that deposit on the deformable surface have, on average, greater velocities than those settling at the flat wall. In particular, for the FDI case, there is a large increase of probability around \( W_p \approx 0.01 \), whereas for the OCH one, the same happens for values of velocity ten times lower. The second part of the curves (on the right side of the plot), for \( \text{St}=15 \), are fairly overlapping, suggesting similarities in this range of velocities between the OCH and the FDI case. The figure suggests the possibility of dividing the population of sampled velocities into two groups:

- Population A: Low velocities
- Population B: High velocities
Figure 4.21: Cumulative Distribution Function of the normal velocity for settling particles.

The division is necessarily arbitrary, but the distribution shown in Fig. 4.21 clearly pleads for a net separation between the two groups. For clarity, Table 4.5 summarizes the way the population has been divided.

<table>
<thead>
<tr>
<th></th>
<th>St=5, OCH</th>
<th>St=15, OCH</th>
<th>St=5, FDI</th>
<th>St=15, FDI</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pop. A</td>
<td>90% (&lt; 0.001)</td>
<td>65% (&lt; 0.002)</td>
<td>97% (&gt; 0.001; &lt; 0.02)</td>
<td>65% (&gt; 0.01; &lt; 0.02)</td>
</tr>
<tr>
<td>Pop. B</td>
<td>10% (&gt; 0.1)</td>
<td>35% (&gt; 0.02)</td>
<td>1% (&gt; 0.1)</td>
<td>25% (&gt; 0.05)</td>
</tr>
</tbody>
</table>

Table 4.5: Typical velocities of depositing particles

Each cell reports the percentage covered by the considered population and the range of velocities characteristic of the group. Note that there are ranges of velocities not covered neither by A nor by B, but their contribution can be neglected for the purpose of this discussion. Although the values are only quantitative, some useful considerations can be made:

1. Population A accounts for most of the velocities in every case.

2. The deviation between A and B percentage is less marked for St=15 than for St=5.

3. The separation between population A and B is more stressed for OCH than for FDI.

4. The relationship between the percentage of the two populations is almost
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Figure 4.22: Probability Distribution Function of the normal velocity for settling particles; OCH case.

The last observation suggests that the mechanism of deposition could be the same for the two cases (FDI and OCH), with velocities that are shifted towards higher values for FDI case.

Figures 4.22 and 4.23 show the Probability Distribution Function (PDF) for normal velocities of the deposited particles. The peak correspond to velocity values around \(1 \times 10^{-4}\) for St=5 particle and around \(2 \times 10^{-4}\) for St=15 particles. Brooke reported values of velocity 1000 times larger for similar particles. From a statistical point of view their results could be affected by some defects in the simulation procedures. They in fact used a smaller number of particles (16129) than in the present work, released from a plane at \(z^+ = 40\) (relatively close to the wall). The particles were then tracked for 700 non-dimensional time units. Assuming the estimate made in Section 4.1.1 to be valid, the particles are probably affected by the initial conditions for most of their simulation. Moreover, since in their work the particle are not reintroduced into the domain once depositing, particle velocity are not calculated in a steady state condition.

The PDF of velocities in the FDI case, show that the differences between the distribution for the two sets of particles are quite similar, at least in the range of values considered in the plot. This is reflected also in the deposition rate. In fact, in the FDI case, the deposition of St=15 particles is only slightly higher than of St=5 particles.
Fig. 4.24 reports the CDF for the difference between fluid and particle velocities (a measure proportional to the particle Reynolds number at a distance of one radius from the lower boundary). Here, both $W_f$ and $W_p$ are pointing towards the wall/interface. A positive value therefore indicates that a particle is depositing in a zone where the fluid is moving outwards from the wall, since all velocities of depositing particles should be positive. The data confirm the division of population made previously. Most of the particles deposit with a velocity very close to that of the fluid at one particle radius of distance from the boundary (population A), while population B is represented on the left of the curves, not completely shown in the plot (particles depositing with high velocities not characteristic of region adjacent to the wall). One can also notice that, for the FDI case, there is a significant number of particles (25% and 35% for St=15 and St=5, respectively) that deposit against fluid motion (from the interface outwards). The definition of the normal velocity of the fluid typical of the location where deposition occurs (the antithesis of the velocity typical of the bulk flow) requires a discussion. Brooke et al. took the RMS of wall normal fluctuation at one radius of distance from the wall as a characteristic velocity. Their assumption seems to be correct, since there is no mean velocity for the fluid in this direction; the only flow motions in this zone can only be oscillations around zero due to small perturbations. Strong large-scale motions like sweep events hardly reach a distance so close to the wall, even if they control the
In our work, the RMS of normal fluid and particle velocity fluctuation, where the differences between the two boundaries became apparent ($z^+ < 5$) has been analyzed by accounting for Brooke’s suggestion (Fig. 4.25). In these regions the RMS of the particles are higher than the RMS of the fluid. This is surprising since the particle motion is determined by the fluid, and particles presence does not affect turbulence intensity due to the assumption of one-way coupling. A possible explanation is that particles reside on average in zones of higher turbulence fluctuations than the mean at that height (in fact, preferential accumulation is very strong in the region near the lower boundary). The RMS of normal velocity fluctuations is a weak function of the $z$ coordinate for FDI case and has a value around $5 \cdot 10^{-3}$ at the deposition position. For the OCH case, the corresponding value is around $1 \cdot 10^{-4}$. Looking again at Fig.4.22 and Fig. 4.23 reveals that most of the particles deposit with velocities typical of the region adjacent to the lower boundary.

The transport of discrete particles because of the mixing induced by turbulent fluctuations is often referred to as turbulent diffusion. In the same way, population A, accounting for particles that deposit because of small fluctuations near the wall, will be referred to as diffusion-dominated population. This mechanism of deposition is the observed main contribution in the present work. The population of large velocity particles (which in the following will be referred to as free-flight particles), whose deposition is controlled by inertia-dominated mech-
anisms, is however an important contribution, in particular for St=15 particles.

Figure 4.25: Normal RMS values of fluid and particles velocities in the region adjacent to the wall.
4.5 Particle residence time analysis

The previous analysis of the deposition velocities does not explain by itself all the mechanisms and needs further investigation.

From previous discussion, some questions still prevail:

1. From where does the population B acquires such high velocity? In the near wall region adjacent to the wall or at higher locations?

2. How much time does a particle spend near the wall before depositing?

3. Are the two mechanisms of deposition decoupled in time?

To answer these questions, a particle residence time analysis has been conducted. The time spent by a particle in a slab of 3 wall units from the wall before depositing has been recorded. A routine has been implemented in a way that, if a particle escapes from the slab in which it have resided during a certain interval of time (being re-entrained in the bulk flow), the time counter for this particle is reinitialized. Figures 4.26 and 4.27 show a scatter plot relating the particle residence time and the deposition velocity. Logarithmic scales for both axes have been deliberately adopted. The separation between two different populations is now more visible, reinforcing previous results in connection with the distribution of the velocities of deposited particles. Population B, characterized by small residence time and large velocities, is clearly recognizable on the left of the plot. For this particles the relationship between the Logarithm of time and velocity is quasi linear.

The fact that these particles originate from $z^+ > 3$ regions is confirmed by an estimate, based on the assumption that the free-flight particles have velocities high enough to pass the viscous sublayer, without being substantially retarded. In this case, the velocity within the 3 wall units slab could be considered constant.

As a consequence:

$$ W_p \approx \frac{z^*}{t^*} \quad \text{or} \quad \log W_p = \frac{-\log(z^*) \cdot \log(t^*)}{\log(z^*)} $$

where $z^*$ is 3 wall units and $t^*$ the residence time. Since the values calculated with the previous relation agree with those found in the plot, the assumption
advanced in making the estimate is correct. It is important to note that this
does not imply that $z^+ = 3$ is the free-flight distance according to Friedlander’s
analysis, but it only means that this set of particles were initially in regions above
3 wall units distance from the wall/interface. Population A is associated with the
particles on the right side of the plots. The residence times characteristic of this
population are clearly larger than those of population B. Moreover, comparing
the OCH and the FDI cases for the two sets of particles shows the time spent by
a particle before deposing at the deformable interface to be remarkably shorter
than that needed for deposition on the flat wall. Since the RMS of the vertical
velocity fluctuations of the fluid in the region near the interface/wall are higher
for the FDI case, fluid motions strong enough to make a particle deposit are
more frequent in this case and the residence time is lower. In this respect, the
deposition at the deformable interface could be considered as a more efficient
mechanism than in OCH.

As pointed out in Section 4.4.3, the division between the two populations is
not very marked for $St=15$, particularly for the FDI case. This is reflected also
in Fig. 4.27, where intermediate residence times and velocities that can hardly
be attributed to one of the two populations can be noticed.
Figure 4.27: Correlation between the residence time and the velocity of the settling particles (St=15).

Figure 4.28 shows the PDF of the residence time of population B. The analysis of the residence time confirms a previous observation, that is, both considering depositions at the wall and on the deformable interface, the contribution of free-flight particles is more pronounced for St=15 than for St=5.
4.6 Particle concentration patterns

The previous discussion pointed out the importance of preferential concentration mechanisms in affecting velocity statistics of the particle phase. Several animations of the particle field has been carefully examined and it seems that concentration patterns occur everywhere in the domain, both in the bulk flow and near the boundaries.

Figures 4.29–4.32 show perspective views of the particle distribution in the region extending from $x^+ = 2148$ to 3222, at $t^+ = 2390$, for the four cases (approximately 20000 particles are present in this location at that instant). Core flow seems to be less populated in the OCH case than in the FDI configuration. The accumulation of particles for long intervals of times at the lower boundary prevent them to be reintroduced and re-populate the domain. This is particularly true for low Stokes number particles in OCH (which have the largest residence times).

Long and persistent lines of particle patterns are present in the bulk flow. This is an evident characteristic of FDI, while in the OCH case the particle field appears more mixed. However the difference is clearly difficult to quantify. Rouson & Eaton [50] noticed “...lengthy streamwise bands reminiscent of the near wall streaks...” without providing correlation between particle location and local turbulence structure; they concluded that the concentration distribution in the core of the channel was an artifact of structures closer to the wall. In fact, in the experiment of Fessler et al. [18], which they tried to reproduce numerically, no structures resembling streaks were found. Rouson & Eaton observed that the difference might have been due to the lower Reynolds number used in their DNS. In fact, in all numerical experiments at low shear rate, the longitudinal coherent structures that cause segregation occupy large part of the domain height, while in the experiments the boundary layer is so thin that this lines are moving only very close to the wall. This observation holds for the present calculations, too.

In the present simulations the lines seem to form in the core flow, slightly towards the lower boundary in the zone populated by quasi-streamwise vortices. A curious phenomenon has been observed in the present work: the downstream edge of the particle streaks seems to whip towards the free surface. These lines, in particular for the FDI case, persist for quite long periods, but they
periodically break-down as a consequence of strong wall-ward fluid motions. The breaking of the streak is accompanied by the ejection of particles towards the upper boundary. In the FDI case the lines are more continuous, thus this process leads massive clusters of particles to hit the free-slip boundary. This explains the reason why deposition at the free-surface is an intermittent and not a continuous phenomenon (see Section 4.3).

Particle streaks at the wall are one of the most commonly observed feature of boundary layer laden with particles. Analyzing particle distribution in the region adjacent to the wall/interface, shows that the type of boundary used in the FDI simulation changes the characteristics of this lines. Figures 4.33–4.36 show snapshots of particles located in the region $z^+ = 0 − 5$, in order to make distribution at the wall more clear. For the OCH case, the lines are more straight and continuous while in the FDI case the streaks are dispersed and broken in some points. Flow animations have shown that the lines swing and flicker at the wall, a sign of turbulent activity persisting also in the zone immediately adjacent to the lower boundary. Instantaneous correlation between particle lines at the wall and low-speed streaks is a well established fact in wall-bounded particle laden flows (e.g. [42]). This is also present in the flow over a deformable interface as depicted in Figs. 4.37 and 4.38, presenting a top view of the near wall region ($z^+ < 13$). Both sets of particles preferentially concentrate in regions of low streamwise velocity (visualized through contour plots). Even though, the distribution is clearly more dispersed for the high Stokes number particles.
Figure 4.29: Instantaneous particle distribution : 3D View (St=5, OCH).

Figure 4.30: Instantaneous particle distribution : 3D View (St=15, OCH).
Figure 4.31: Instantaneous particle distribution : 3D View (St=5, FDI).

Figure 4.32: Instantaneous particle distribution : 3D View (St=15, FDI).
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Figure 4.33: Particle distribution near the wall (St=5, OCH).

Figure 4.34: Particle distribution near the wall (St=15, OCH).
Figure 4.35: Particle distribution near the wall (St=5, FDI).

Figure 4.36: Particle distribution near the wall (St=15, FDI).
Since low-speed regions perceive the action of streamwise vortices acting near the wall, this correlation means that the mechanisms of particle transport and segregation near the wall might be controlled by coherent fluid motions, also in the FDI case. According to a simple, deterministic view of this phenomenon ([9, 19, 53, 34]), particles are mainly brought to the wall by sweeps and eventually re-engrained through ejections. This two events are clearly three-dimensional, making the movements of the particles engaged into fluid motions difficult to follow in time. However, Figs. 4.39–4.42 show that particles to reach the wall following preferential paths, making the spatial distribution in the cross-plane quasi two-dimensional and well structured.

Through similar avenues, particles reach the upper boundary suggesting similarities between particle transfer mechanisms at the free-slip and no-slip surfaces even if the turbulence characteristics are different. The figures also show that in the OCH case the particle phase is more dispersed and mixed than in the FDI case, where regions completely empty are separated by locations where the
Figure 4.38: Instantaneous correlation between low-speed regions and particle streaks (St=15, FDI).
particle number density is very high.

For completeness, Figs. 4.43–4.46 show a side view \((X - Z \text{ plane})\) taken at the same instant. The particles are disposed following elongated slightly inclined structures that resemble in the shape quasi-streamwise vortices. In snapshots taken at other instants this similarity is even more evident. Considering, for example, Fig. 4.47, it shows a particle structure in the center of the figure with a helicoidal shape that is very similar to the “funnel” shaped vortex depicted in Fig. 4.48 (a sketch taken from Kaftori et al. [28]). In their work, these authors found that this fluid structure can account for most if not all coherent motions observed during years of investigations of wall turbulence phenomena.

Figure 4.49 and 4.50 show time evolution of this streakline of particles. It seems that the particles are engulfed in the fluid structure and follow it being transported with the mean flow. This explains why, in particular for the FDI case, particle streaks are relatively long-lived (as the streamwise coherent structures) and quite continuous. As already pointed out, in fact, the fluid structures that populate the boundary layer are more elongated and more streamwise oriented in this latter case. Imagine that the underlying fluid vortex is convected downstream with the mean flow (whose direction is indicated with an arrow), its head pointing upstream towards the free surface and oscillating up and down, while the narrow opening is always very close to the wall. This is the typical behaviour of a funnel vortex in Kaftori’s observations. If the oscillations of the fluid structures in the normal direction have long characteristic times, the particles engulfed in it can follow fluid motion, maintaining spatial coherence. Sometimes sudden strong fluid motions towards the wall disrupt the particle cluster. The resulting effect is that the line of particles breaks (Fig.4.49) in two sections. The particles which belong to the upstream part collect at the wall, while the others follow the bulk fluid motions and reach the upper boundary. This is another view of the process already described at the beginning of this section.

Once the particles reach the region near the upper boundary, they are subjected to the large scale structures characteristic of free surface turbulence (see Section 2.1). In both experiments [30] and DNS [59], the formation of roughly circular particle concentration patterns has been observed in this location. Fig-
Figure 4.51 shows these structures as observed in our OCH simulation. Actually, the concentration of particles is not high enough to make the contours clear. In FDI the structures are more elongated (Fig. 4.52). In this case, the particles reside near the free surface during a shorter period than in the OCH case. Consequently, they have no time to react to the large-scale turbulent structures populating these regions.
Figure 4.39: Cross section view of particle distribution (St=5, OCH)

Figure 4.40: Cross section view of particle distribution (St=15, OCH).
Figure 4.41: Cross section view of particle distribution (St=5, FDI).

Figure 4.42: Cross section view of particle distribution (St=15, FDI).
Figure 4.43: Instantaneous particle distribution: side view (St=5, OCH).

Figure 4.44: Instantaneous particle distribution: side view (St=15, OCH).

Figure 4.45: Instantaneous particle distribution: side view (St=5, FDI).

Figure 4.46: Instantaneous particle distribution: side view (St=15, FDI).
Figure 4.47: Time progression of a ribbon shaped particle streak: first instant (St=5, FDI).

Figure 4.48: Sketch of a funnel vortex.

Figure 4.49: Time progression of a ribbon shaped particle streak: second instant (St=5, FDI).

Figure 4.50: Time progression of a ribbon shaped particle streak: third instant (St=5, FDI).
Figure 4.51: Particle distribution near the free surface in the OCH case; (a) St=5, (b) St=15.

Figure 4.52: Particle distribution near the free surface in the FDI case; (a) St=5, (b) St=15.
4.7 Preferential deposition

In order to give a complete description of the preferential accumulation phenomena observed in the present work, it would be interesting to look at where exactly the particle tend to deposit at the lower boundary. At every time-step, only a few particle deposit, hence no preferential zones can be noticed with instantaneous snapshots. Figures. 4.53–4.56 visualize where the particles have deposited over an (X-Y) plane located at one radius of distance from the wall/interface, during the whole simulation (i.e. all the settled particles are included in the scatter plot since, at every time-step, only a few particle deposit, hence no preferential zones can be noticed with instantaneous snapshots). This can be considered a density plot of the probability that a particle deposits at a certain position at the lower boundary. Particles colored in blue are particles that deposit with high normal velocities (i.e. more than a cut-off velocity equal to 0.02), those colored in red have velocities less than 0.02. The cut-off velocity value has been taken arbitrarily, but in a way to roughly divide the population of deposited particles into free-flight particles (blue) and diffusion-dominated particles (red).

The examination of the distribution, in the OCH case, leads to the conclusion that low deposition-velocity particles deposit preferentially in streaks while free-flight ones are well distributed over the whole plane. This is not surprising, since diffusion dominated particles come from locations very close to the lower boundary, where particles have already accumulated in streaks. This massive rows of particles are moving in a quasi-quiescent environment and are not well mixed, so they drop particles only near their location. Consequently, particle distribution at the deposition position trace clearly the near wall particle distribution. Instead, particles with high velocity come from the bulk flow, where the dispersed phase is better mixed: large scale, coherent fluid motions are moving in the bulk region with the mean flow, flinging particles evenly to the wall.

In the FDI case particle position is not as related to the deposition velocity as in the OCH case. As already pointed out, the distinction between the free-flight particles and the diffusion dominated particles is not as marked as in the OCH case, at least when based on the velocity distribution. The two populations have characteristic values of wall-normal velocity quite close and it is difficult
to show the division visually. However, it seems that high velocity particles are more dispersed over the (X-Y) plane in this case too.

The turbulence properties at the lower boundary are strongly affected by the presence of the capillary waves. In particular, De Angelis et al. [14] noticed that high shear stresses correspond to the crest, and low shear to the valleys of the waves. Moreover, these authors pointed out that the waves do not seem to affect the kinematics of the flow. Sweeps are correlated with regions of high shear stress and ejections are more probable for low shear stress (as in the flow over flat plane). The mechanisms of particle segregation near the wall are
Figure 4.55: Particle distribution at the deposition plane (St=5, FDI).

Figure 4.56: Particle distribution at the deposition plane (St=15, FDI).
strongly related to these two events, as shown by many authors ([42, 54, 5, 44]). Moreover in Section 4.4 it has been noticed that an important contribution to deposition is due to particle that deposit, on the free deformable interface, against fluid that is moving outwards from the boundary. Fluid motions induced by ejections events hardly originate from one particle radius of distance from the wall, so this is the effect of the moving surface which force fluid to have a positive normal velocity in some parts of the waves. Boersma [7], in a direct numerical simulation of particle dispersion over a wavy wall, noticed positive normal velocity just upstream of the wave crest. Previous observations suggest that there might exist a correlation between the particle deposition-position and peaks or valleys of the waves of the deformable interface. In Fig. 4.57 the probability distribution function of particle number density shows that the position where the particles deposit and zones where the displacement of the surface is positive are strictly interconnected, for both sets of particles. Positive displacement are, trivially, more probably associated with the peaks than the valleys of the waves. The deposition is, moreover, best correlated with zones where the surface is moving towards the center of the domain (i.e. with positive velocity), as shown in Fig. 4.57.
Figure 4.57: Correlation between surface displacement and deposition position. Surface displacement is scaled with half the height of the channel ($h$).

Figure 4.58: Correlation between surface velocity and deposition position. Surface velocity is scaled with the friction velocity ($u_\ast$).
4.8 Remarks

Figure 4.59: Schematic description of the envisioned two-stage deposition process.

The aim of this section is to try to link together the observations made before. The mechanisms of particle transfer to the wall is still an open subject, and it is even complicated by the presence of a boundary that is free to deform, whose influence on the turbulence properties of the flow is still under investigation in the scientific community. Hence, a great deal of intuition, supported by the experience achieved through visualizations and animation of the particle phase, is necessary in interpreting the results.

The overall picture that the previous analysis suggest is that the particles are deposited at the wall in a two-stage process (Fig. 4.59). Through a turbulent convective mechanism particles reach the region adjacent to the boundaries coming from the bulk flow. This mechanism is very efficient, involving strong and coherent motions of fluid towards the wall that are likely to be the sweep events. The importance of the near wall coherent structure in this respect is remarkable, both in generating these events and in entrapping the particles in streaks causing preferential concentration. Through this mechanism, that has its counterpart in the ‘turbophoretic effect’ (from a modeling point of view), particles reach the viscous sublayer and accumulate there. Considering the statistics for the continuous phase, there is no reason to believe that this first-stage mechanism is different between the FDI and the OCH case. Moreover, since fourth quadrant events are strong, this process might not be very dependent on particle inertia (i.e. the flux of St=5 particle transported is approximatively the same as that for the St=15 particles). This observation has been confirmed quantitatively in a recent work of Marchioli et al. [34], who showed that the flux of particles
towards the wall for $St=3.8$ and $St=29.1$ is similar.

Once the particles reach the region adjacent to the wall, their history can follow two different paths. The “free-flight” particles are those which continue their motion towards the wall without being substantially decelerated and immediately deposit. It is more probable that, because of its larger inertia, a $St=15$ particle deposits with this mechanism. The other particles (i.e. diffusion dominated particles) accumulate for relatively long times, depositing because of random, weak fluctuations near the wall. The residence time analysis for the OCH case shows that this two stages are clearly decoupled in time for the diffusion dominated particles, while they constitute quite a continuous process for the particles that deposit in free-flight.

In Fig. 4.59 this two-stage mechanism is rendered in a schematic way. The length of the arrows is proportional to the time-length that characterize the phenomenon and their depth is proportional to the relative contribution to the total deposition. For the FDI case, since the diffusion dominated particles deposit in shorter times, the second stage of the process of deposition follow more directly the first (as far as regards the time progression). In fact, the particles are transported in the viscous sublayer, where they find a region more active in turbulent fluctuations than in the wall bounded flow. As a consequence, the diffusion dominated particles deposit quite rapidly and with a bigger vertical velocity than in the OCH case. Because of this, the division between the two populations is less marked. The physical processes that make them deposit are separated, but, just from the statistics of the velocity and residence time distribution of the deposited particles, this division is not as evident as in the OCH case (probably the two populations are partially overlapping). According to this scenario, the fact that particles deposit preferentially on the peaks of the waves is explained by the presence of high shear stress at these positions. Particle transported towards the wall by sweeps (producing shear) will deposit preferentially in regions of positive displacement.

Previous observations help in understanding why the deposition rate for the $St=5$ particles is very close to that of the $St=15$ particles in the FDI case. From a physical point of view this is the consequence of the fact that, for both sets, the particles coming from the bulk region reach the near interface region
because of a mechanism that is quite independent on particle inertia, being
due to strong fluid motions (i.e. the accumulation stage). Moreover, the further
process, which leads the particles to deposit, is more time-coupled for the FDI
than in the OCH case, so the flux of particles coming from the bulk flow is
quantitatively very close to the flux of particle that deposit.

Considering the same process in statistical terms, the observed deposition
rate is explained taking in account two observations:

- The number of particle that deposit because of the diffusion mechanism
  is a quantity that depends on the type of boundary considered (free de-
  formable interface or wall), because it is mainly caused by small fluctuation
  near the boundary.

- The contribution of the free-flight particles coming from the bulk flow to-
  wards the lower boundary is expected to be approximatively independent
  of the type of boundary.

Almost all the light particles (St=5) deposit because of the first mechanism.
As a consequence the increase in deposition passing from the OCH to the FDI
case is very large. On the contrary, for the St=15 particles, the free-flight
mechanism is an important contribution and the increase in deposition is less
marked. However, evaluating the relative importance of the two contributions
from a quantitative point of view, is not straightforward, because of the afore-
mentioned difficulty to divide, using a simple criterion, the two populations in
the FDI case.
4.9 Summary

A detailed analysis of the simulations has been performed in order to compare the particle field properties in the OCH and in the FDI case. It has been noticed that particles tend to accumulate in the viscous sublayer. This build-up of particles is bigger for the OCH case, in particular for the light particles. The concentration gradient near the wall has been found smoother in the case of particle dispersion over the deformable interface than over the flat wall.

The particle velocity statistics in the bulk flow have not shown remarkable differences between the two cases. The results are overall quite satisfactory, considering that some disagreements with data found in literature have been explained considering the phenomenon of preferential concentration, which strongly influences the statistical characterization of the particle velocity field. It has been observed that particle clustering occurs both in the near wall/interface region and in the bulk flow and it has been associated to the action of the quasi-streamwise vortices populating the boundary layer.

The deposition coefficients for both the cases have been calculated. The agreement between the deposition rates predicted by the current simulation and previous works have been found to be satisfactory for the OCH case. The presence of the free-deformable interface enhances the deposition of the particles. The increase is remarkable for the St=5 particles while is only significant for the St=15 ones. A division of the population of deposited particles, based on the probability distribution of the particle deposition velocity, has been proposed, and the results validated with an analysis of the residence time near the wall. It has been proved that the majority of the particles deposit because of small, random fluctuations near the wall, while a minor contribution is constituted by particles that come with high velocity from the bulk-flow. An attempt has been made to connect the physical process that make the particle accumulate in the near wall region to the mechanism that causes them to actually deposit. These two mechanisms have been found to be strongly decoupled for the OCH, while for the FDI case they constitutes a more continuous process. A statistical interpretation of the observed deposition rate has been considered, too.
Chapter 5

SUMMARY AND CONCLUSIONS

In this work a Lagrangian particle tracking at low Reynolds number has been performed. The turbulent flow where the particles are tracked is the gas side of a counter-current air water flow, in which the two immiscible phases are separated by an interface that is free to deform under the effect of the shear due to the relative motion. The dispersion of two sets of particles, with Stokes numbers equal to 5 and 15, has been studied. In order to obtain a fully developed particle field a suitable computational procedure has been carefully selected. This approach consists of removing particles reaching the boundaries and reintroducing them at the inflow plane.

The main objective of this work was trying to assess the differences between the particle dispersion in the flow over a deformable interface and in a conventional open channel flow. For this purpose, a further Lagrangian particle tracking simulation has been performed. In this case the numerical parameters and the set of particles has been kept the same, while the continuous phase properties were different (i.e. flow over flat plane). The particle phase velocity field has not been found significantly affected by the different boundary conditions in the bulk flow. As expected, remarkable differences near the wall INTERFACE has been noticed between the velocity distributions of the particles in the two cases. In particular the RMS values of normal velocity fluctuations for the particles
have been found much greater for the flow over the deformable interface than for the flow over the flat plane. The deposition coefficients for the two cases have been compared and it has been concluded that the presence of the deformable interface considerably enhanced the deposition of small inertia particles, while the increase is only slight for the St=15 particles. The particle concentration field in the normal direction has been found strongly affected by the presence of the deformable boundary; in particular, both the gradient and the peak value of the normal particle concentration distribution are smaller near the interface than near the wall. It has been observed, moreover, that phenomena of particle clustering occur both in the bulk flow and in the viscous sublayer, and that this effect seems to be stronger for the flow over the deformable interface. A division of the population of the deposited particles based on the statistical characterization of the particle deposition velocity has been proposed and the results confirmed with the analysis of the time spent by the particles in the near wall-region before depositing. It has been proved that the majority of the particles deposit because of turbulent fluctuations near the wall (turbulent diffusion); an inertia-dominated mechanism (free-flight) is however an important contribution for the St=15 particles. A physical and statistical interpretation of the observed deposition rate has been proposed, which envisions a two-stage particle transfer mechanism.

The analysis performed show clearly that different boundary conditions for the flow (in this case flat plane and deformable interface) could affect strongly the statistic for the dispersed phase that are related to near wall/interface phenomena, in particular the deposition rate. This, in turn, could change the particle concentration field remarkably, in spite of the fact that turbulence characteristics in the bulk flow are not significantly different.

The project was very ambitious, so several suggestion for future work resulted from the current investigation. These recommendations could be listed as follow:

- Quantify the differences in the observed preferential concentration phenomena between the two cases, using objective measures (see [22]), and study their dependence on the Stokes number.

- Focusing on the FDI case and considering a larger set of particles, study
how the deposition coefficient changes as a function of the particle response time.

- Define a more rigorous and less arbitrary criterion to divide the population of deposited particle in free-flight and diffusion dominated particles. The one proposed is useful in the wall-bounded particle laden flow but it has some shortcomings when applied to studies of particle dispersion over a deformable interface.

- Investigate further the relation between the physical interpretation of the phenomenon of particle accumulation (based on the sweep-ejection cycle) and the statistical characterization of the deposition mechanism.
Bibliography


