

Direct numerical simulation of monodisperse fluid-particle flows

Methodology, validation, and application to fixed and
fluidized beds

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À Maman.

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Introduction

Context

Flows where a dispersed solid phase is transported by a carrier fluid are encountered both in environmental phenomena and industrial applications. They are broadly referred to as particle-laden flows. In nature, the dispersion of ashes in the plume of a volcano or the transport of sediments in a river may have sanitary or environmental consequences that need to be managed. In the industry, fluidized beds are used in numerous processes in petrochemicals (fluid catalytic cracking) in the pharmaceutical sector, in energy conversion (biomass pyrolysis), in CO₂-capture applications (chemical looping combustion) or in the food industry, among others. They owe their popularity to the intense mixing provided by the fluidization of the particles under the action of an upflowing fluid, resulting in unique heat and mass transfer properties.

In particle-laden flows, the interplay between the fluid-particle and the particle-particle interactions leads to a wide variety of regimes and to a rich physics characterized by complex multiscale structures ranging from the dimension of the equipment (i.e. order of meters) to the particle size at the sub-millimeter scale. It is common to classify the different physical scales as follows [118]: (i) the micro-scale representing structures with a size $\mathcal{O}((1 - 10)d_p)$, where d_p is the particle diameter, (ii) the meso-scale representing structures with a size $\mathcal{O}((10 - 100)d_p)$ and (iii) the macro-scale representing structures with a size similar to the size of the equipment. This wide range of scales makes the modeling of fluid-particle flows particularly challenging and explains why the design of fluidized beds is still mostly based on empirical methods.

Multiscale modeling strategy of particle flows

In the last decades, numerical simulation has become a valuable tool to obtain a better understanding of these flows and assist the design, scale-up and operation of fluidized beds. Despite the progress of computational resources, it is still not possible (nor will it be in a foreseeable future) to use a single method capable of capturing all the time and length scales. A multiscale modeling strategy is now well established in the particle-laden flows community where small-scale models are used to develop closure laws that can represent the net effect of the interactions unresolved in larger-scale models [142]. The global picture of this multiscale approach is illustrated in Figure A.

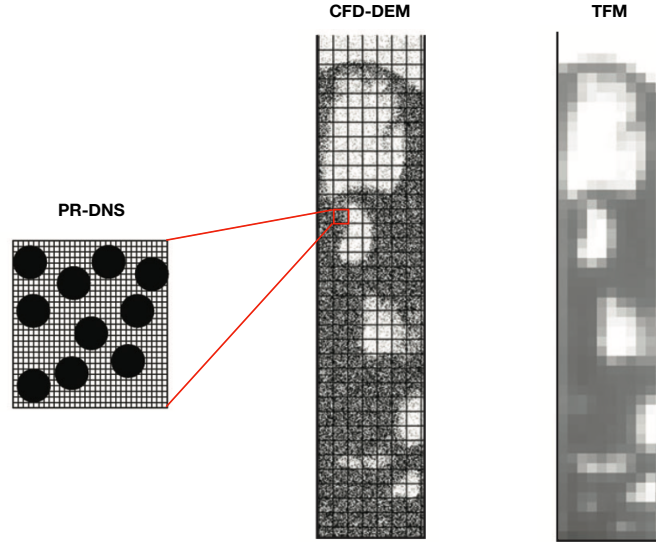


Figure A: Multiscale modeling strategy in particle-laden flows. Image reproduced from [142].

At the micro-scale, particle-resolved direct numerical simulations (PR-DNS or PRS) solve explicitly the fluid-particle and the particle-particle interactions. The fluid-phase is solved in an Eulerian frame and the mesh size h is at least one order of magnitude smaller than the particle diameter in order to capture the smallest flow details and the interfacial stresses. For the solid phase, a Discrete Element Method (DEM) [20] is generally used: particles are tracked in a Lagrangian fashion by solving the Newton-Euler equations of motion and particle-particle interactions are handled by a contact

force model, either a hard-sphere or a soft-sphere model (more details concerning collision models are provided in Appendix A). Since PR-DNS methods derive from first principles (mass, momentum and energy conservation at the smallest scale), they do not require any closure modeling. Yet, they differ in the strategy used to impose the boundary conditions at the fluid-solid interface, as discussed below. This kind of approach is still limited to systems containing $\mathcal{O}(10^3 - 10^4)$ particles, although some recent studies report the simulation of 10^5 resolved particles [57]; and even up to 10^6 particles when using many GPUs [154]. However, these simulations are restricted to academic uses and require an extensive amount of resources.

At the meso-scale, (unresolved) Euler-Lagrange (EL) methods take a similar approach: the fluid phase is solved on a Eulerian grid and the solid phase is handled by a DEM. However, the Eulerian grid size in this approach is generally an order of magnitude larger than the particle size. The fluid-particle interactions (i.e. mass, momentum and heat fluxes) are no longer captured by the simulation and closure laws must be provided to achieve the coupling between the two phases. With this approach, also referred to as CFD-DEM, lab-scale equipments containing $\mathcal{O}(10^6)$ to $\mathcal{O}(10^8)$ particles can be tackled [17, 30].

At the macro-scale, and for industrial-size devices containing $\mathcal{O}(10^9)$ particles, the Lagrangian tracking of the solid phase becomes impractical. In the Euler-Euler (EE) approach, or Two-Fluid Model (TFM), the fluid and the solid phases are treated as interpenetrating continua whose governing equations are solved on the same Eulerian grid [48, 114]. The concept of individual particles has disappeared and the solid phase is identified by a volume fraction field. The TFM equations can be either postulated from the mixture theory [7] or rigorously derived by volume-averaging [5, 59] or ensemble-averaging [29] of the micro-scale equations. Similar to the EL approach, closure laws are needed to model the unresolved fluid-particle interactions. In addition, since the solid phase is treated as a continuum, closure laws must also be provided for the pressure and the shear stress tensor that appear in the momentum conservation equation of the solid phase. Most recent models rely on closures obtained from the kinetic theory of granular flows (KTGF) [61, 28].

Numerical methods for particle-resolved simulations

The main challenges in particle resolved simulations are (i) correctly enforcing the boundary conditions needed to solve the fluid-phase governing equations and (ii) evaluating the interfacial stresses to update the motion of the solid particles. A graphical summary of the diversity of methods used in particle resolved simulations is presented

in Figure B. A first distinction is made between the methods that rely on a body-fitted grid and those that use a fixed, non conformal grid.

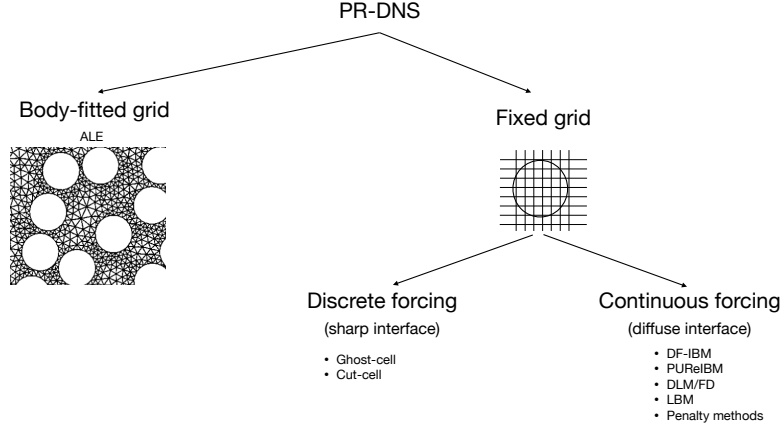


Figure B: Classification of the main methods used to perform resolved simulations of particle flows. Body-fitted mesh figure has been reproduced from [58].

Methods based on a body-fitted (or conformal) grid such as the arbitrary Lagrangian-Eulerian (ALE) finite-element method [58] allow a straightforward treatment of the boundary conditions in the discretization process of the governing equations. However, complex geometries or systems with a large fraction of the domain occupied by the dispersed phase make the meshing process increasingly difficult. Most of all, the treatment of moving bodies requires a remeshing procedure at each time step and a projection of the solution onto the new grid. These two operations drastically increase the complexity and the computational cost of the numerical method.

Conversely, methods employing a fixed (usually Cartesian) grid can produce fast solutions for systems with moving bodies. However, since the Eulerian grid no longer conforms to the boundaries of the obstacles in the flow, an effort is needed to properly impose the boundary conditions on the surface of the particles. Among those methods, a distinction is made between continuous forcing and discrete forcing approaches [87]. In the continuous forcing approach, the enforcement of the boundary condition is performed by modifying the continuous expression of the Navier-Stokes equations, usually by the addition of a forcing term (see details in Chapter 1). Those methods

always introduce some mollification of the interface, so that the spatial accuracy of the method is generally reduced to first order. In the discrete forcing approach, the presence of the interface is introduced after discretizing the original Navier-Stokes equations, i.e. at the level of the discrete differential spatial operators. These methods keep a sharp representation of the interface but they are also much more intrusive from a numerical development perspective. Among those sharp interface methods, the ghost-cell [79, 138, 23] and the cut-cell approaches [139, 85] are the two most popular. In the former approach, a ghost cell refers to a grid cell located in the solid phase and that has at least one neighbor cell in the fluid phase. The value of a ghost cell is determined by the boundary condition and by extrapolating the solution fields from the fluid phase (several schemes have been derived by Majumdar et al. [79]). In the cut-cell approach, each fluid cell crossed by the interface is reshaped, discarding the part of the cell lying in the solid. The result of this operation is the creation of trapezoidal control volumes, leading to a finite-volume discretization of the Navier-Stokes equations.

The first continuous immersed boundary method (IBM) was developed by Peskin [98] to simulate flexible blood vessels. The direct-forcing (DF) version of the IBM was introduced by Mohd-Yusof [88], with the forcing term being evaluated on discrete Lagrangian points using the boundary condition and the discretized form of the transport equations. A comprehensive formulation of the DF-IBM for particle flows was later proposed by Uhlmann [141] and subsequently improved by several researchers [65, 15, 76], as detailed in Chapter 1. A downside of the DF-IBM lies in the over-estimation of the hydrodynamic radius (i.e. the effective radius "seen" by the fluid) due to the interpolation-spreading operations needed to evaluate the forcing term. To solve this problem, Subramaniam and co-workers [132, 134, 133, 120, 121] proposed their Particle-resolved Uncontaminated fluid Reconcilable Immersed Boundary Method (PUREIBM) where the forcing term is only applied in a thin layer inside the body. Another category of methods originate from the Discrete Lagrange Multiplier / Fictitious Domain (DLM/FD) method introduced by Glowinski [50, 51] in a finite element framework and subsequently used by numerous researchers [96, 146, 148, 159]. In this approach, the use of Lagrange multipliers constrains the flow inside the particles to have a rigid-body motion and the solid and fluid phases are solved in a coupled fashion. Sharma and Patankar [112] extended the DLM/FD method to a finite volume / staggered grid framework. More recently Vincent et al. [145] proposed an implicit tensorial penalty method (ITPM), based on a specific decomposition of the stress tensor in order to impose the correct constraint on the flow inside the particles. A noticeable contribution comes from the Physalis method developed by Prosperetti and co-workers [101, 113]. The problem of the boundary condition enforcement is solved by using

analytical solutions for the flow that are valid in the immediate neighborhood of the particles and that act as a bridge between the particle surface and the rest of the flow. Finally, we must mention some of the numerous studies regarding fluid-particle flows that employ the Lattice-Boltzmann Method (LBM) to solve the fluid phase [143, 9]. Feng and Michaelides also coupled the LBM with the direct forcing approach to enforce the boundary condition on the particle surface [42].

Resolved simulations have thus been used for several years now to explore different features of particle-laden flows. A more complete inventory of recent achievements using PR-DNS is made progressively as we move forward in this work.

Thesis objectives

Given the novelty of this topic in our research group, a significant effort will be devoted to establishing a reliable and efficient computational framework for the study of particle-laden flows. Hence, a first objective of this work will be the development of a robust immersed boundary method to perform resolved simulations of fluid-particle flows in three dimensions. The scope of this thesis will be limited to monodisperse systems, i.e. consisting of same-size spherical particles. Additional physical phenomena such as heat and mass transfer between the two phases as well as natural convection effects should also be included. The methodology developed in this work proves to be capable of performing state-of-the-art calculations in an efficient manner.

As discussed above, the resolved simulation of particle flows offers a unique level of details at the cost of important calculation resources. In particular, capturing the flow in the interstitial spaces between the particles gives access to the local fluctuations of all the fluid and solid phase quantities (velocities, stresses, fluxes). From a statistical point of view, PR-DNS can be considered to reconstruct the complete distribution of any quantity of interest defined in either phase. Yet, the accuracy of the reconstruction of these distributions from a realization of the flow is dependent on the dimensions of the computational domain and on the number of particles in the system. In the last years, PR-DNS has been quite widely used to extract the average value of fluid-particle interactions (i.e. the first moment of their distribution), namely the mean fluid-particle force and heat flux, for a wide range of macroscopic parameters. Those data have then been used to build "first-principles based" closures in terms of drag coefficient and Nusselt number in order to replace the still widely used empirical correlations. However, few studies have explored the richness of PR-DNS to characterize in greater details the distribution of those quantities. Hence a second objective of this work will be to characterize and potentially predict the distribution of the fluid-particle

force and the fluid-particle heat flux in fixed particle systems. To that end, this study proposes one of the first explicit microstructure-based models to predict the fluid force experienced by a given particle from the local organization of the particles in its neighborhood. This advance overcomes the current average drag description and will open the way for microstructure-informed CFD-DEM simulations.

Another question that arises is the validity of extrapolating the conclusions drawn from results obtained on static configurations to systems with freely moving particles. In particular, fixed particle arrays correspond to systems with infinite inertia while free suspensions are allowed to adapt to the flow. It is still not clear in the literature how the agitation of the particles affects the mean fluid-particle force and heat flux, as well as the distribution of those quantities relatively to their mean. Hence, a third objective will be to study small-scale fluidized beds in order to characterize their dynamics and explore statistics that are unavailable otherwise. Different flow regimes will be investigated and a comparison with the results obtained for fixed particle systems will be performed. The sensitivity of our PR-DNS results to some numerical parameters will also be addressed.

Thesis outline

In Chapter 1, we present the direct-forcing immersed boundary method developed in this work. Once the numerical details are presented, a thorough validation campaign is conducted in two- and three-dimensions. Finally, the parallelization strategy of our method in the 3-D solver is detailed and its scaling performance is demonstrated.

In Chapter 2, the method is employed to study the distribution of the fluid-particle force when a fluid flows through randomly distributed arrays of particles. We first highlight the non-negligible distribution of the force around its mean value, showing the influence of the local neighborhood of the particle on the force it experiences. Then, we propose to characterize the microstructure formed by a particle and its neighbors using a few quantities inspired from the so-called "fabric" tensor. Significant correlations are identified between the fluid-particle force and a few microstructure characteristic quantities. A microstructure-based model for the fluid-particle force is then proposed and evaluated against independent test cases.

Chapter 3 focuses on the heat transfer in the flow past fixed random arrays. We investigate how our PR-DNS data can be used to evaluate the mean interfacial heat flux between the solid and the fluid phases, but also the pseudo-turbulent heat flux that results from the correlation between the temperature and the velocity fields at

micro-scale. The thermal saturation problem is discussed, as well as its impact on the distribution of the fluid-particle heat flux and particle Nusselt number.

Chapter 4 is dedicated to the study of small-scale, dense fluidized beds. We first examine the settling of homogeneous suspensions and validate the ability of our method to handle systems with freely moving particles. Then, the hydrodynamics of liquid-solid fluidized beds is thoroughly studied by performing resolved simulations at different superficial velocities. The distribution of the fluid-particle force is characterized in details and is also compared to the results obtained for fixed particle arrays. The thermal problem is then investigated. In a last section, we study gas-solid fluidized beds with much larger density ratios. The emergence of heterogeneous structures is characterized, and the sensitivity of the results on the transverse dimensions of the domain is discussed. The impact of the presence of solid walls is also addressed.

Finally, we close this manuscript with our conclusions, achievements and perspectives.

Development and validation of a direct-forcing immersed boundary method for fluid-particle flows

1.1 Introduction

The original direct-forcing immersed boundary method (DF-IBM) proposed by Uhlmann [141] has become a popular tool to perform fully resolved simulations of incompressible particle flows, in particular due its relatively easy integration into a finite-volume / fractional-step framework. The method is based on the use of two distinct grids: a fixed Cartesian grid for the fluid and a moving grid attached to the immersed bodies. The transfer of quantities between these two grids is performed using interpolation kernels. As with other continuous forcing methods, the fluid-solid coupling, i.e. the enforcement of the boundary condition at the interface, is achieved by the addition of a forcing term in the momentum conservation equation for the fluid. The hydrodynamic forces can be conveniently evaluated from the IBM forcing term and then used to track the motion of the solid particles in a Lagrangian fashion.

Several modifications and improvements to the original method have been proposed by different authors. Among others, we should mention the important efforts made to improve the accuracy of the boundary condition enforcement ([76, 65, 15]) and to achieve a stronger coupling of the fluid-structure interaction ([155, 137]). The latter issue is motivated by the weak coupling of the original method and its difficulty to handle cases with a low solid-fluid density ratio. The IBM has also been extended to include heat and mass transfer between the fluid and the immersed particles [43, 126, 92].

Our implementation is more specifically based on the improved immersed boundary method proposed by Breugem [15].

In this chapter, we first present the governing equations for the fluid and solid phases and the details of the numerical method. The different features of the method are then thoroughly validated using two- and three-dimensional test cases. In particular, we investigate fixed and mobile configurations with fluid-structure interaction for isothermal particle flows, as well as cases where natural convection plays a role. Finally, we detail the parallelization strategy of the solid solver in 3-D since an efficient parallelization of both the fluid and solid solvers is required to perform resolved simulations of a large ($> \mathcal{O}(10^3)$) number of particles.

1.2 Numerical modeling

1.2.1 Governing equations

Figure 1.1 sketches the computational domain of volume V divided into a fluid sub-domain of volume V_f and a solid sub-domain of volume V_s . The solid sub-domain consists of the ensemble of N_p immersed particles:

$$V_s = \sum_{k=1}^{N_p} V_p^{(k)}, \quad (1.1)$$

where $V_p^{(k)}$ is the volume of the k th particle. Like other fictitious domain (FD) meth-

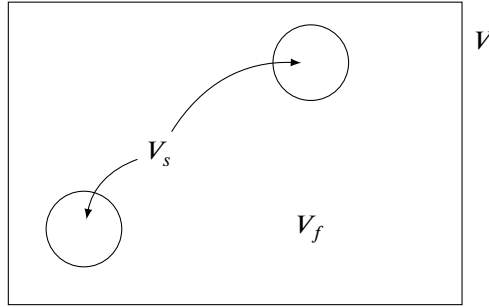


Figure 1.1: Sketch of the computational domain.

ods, the governing equations are solved over the entire domain and the interior of the particles is filled with a "fictitious" fluid of the same density as the real fluid.

Fluid phase

The fluid is assumed incompressible, with density ρ_f . The Boussinesq approximation is used to account for density variations in the buoyancy term, namely

$$\rho_f = \rho_{f_0} (1 - \beta(T - T_0)), \quad (1.2)$$

with the reference temperature T_0 , the reference density ρ_{f_0} ¹ and the fluid expansion coefficient $\beta = -\frac{1}{\rho_{f_0}} \left(\frac{\partial \rho_f}{\partial T} \right) \Big|_{T_0}$.

Assuming constant physical properties, the conservation equations for mass, momentum, energy and species transport in the fluid are given by

$$\nabla \cdot \mathbf{u} = 0 \quad (1.3a)$$

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = \nu \nabla^2 \mathbf{u} - \frac{1}{\rho_{f_0}} \nabla p - \beta(T - T_0) \mathbf{g} + \mathbf{f} \quad (1.3b)$$

$$\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T = \alpha_f \nabla^2 T + S_T + q \quad (1.3c)$$

$$\frac{\partial C_\alpha}{\partial t} + \mathbf{u} \cdot \nabla C_\alpha = D_{\alpha,f} \nabla^2 C_\alpha + S_\alpha + j_\alpha, \quad (1.3d)$$

where $\mathbf{u}$, p , T and C_α are the velocity, the dynamic pressure (i.e. the pressure minus the hydrostatic contribution), the temperature and the species concentration fields ($\alpha = 1, \dots, N_s$ for N_s transported species), $\mathbf{g}$ is the gravitational acceleration, $\nu = \frac{\mu}{\rho_{f_0}}$ is the kinematic viscosity (μ being the dynamic viscosity), $\alpha_f = \frac{k_f}{\rho_{f_0} c_{p_f}}$ is the fluid thermal diffusivity (k_f and c_{p_f} being the fluid thermal conductivity and heat capacity, respectively), $D_{\alpha,f}$ is the diffusivity of species α in the fluid and S_T and S_α are possible energy and species source terms (e.g. resulting from a chemical reaction). To simply notations, the buoyancy term $-\beta(T - T_0)\mathbf{g}$ will be noted $\mathbf{B}$. The additional terms $\mathbf{f}$, q and j_α are the IBM momentum, energy and species forcing terms added to satisfy the corresponding Dirichlet boundary conditions at the surface of the particles.

The solid particles are assumed to be perfectly rigid. Hence, a material point in the solid phase with position vector $\mathbf{X} \in V_p$ has a velocity vector $\mathbf{U}_p$ given by

$$\mathbf{U}_p(\mathbf{X}) = \mathbf{u}_p + \boldsymbol{\Omega}_p \wedge \mathbf{r}, \quad (1.4)$$

where $\mathbf{u}_p$ is the center-of-mass velocity of the particle, $\boldsymbol{\Omega}_p$ its angular velocity and $\mathbf{r} = \mathbf{X} - \mathbf{x}_p$ the position of the material point relatively to the centroid of the particle,

¹When it is made clear that no natural convection effects are at play in the problem considered, the uniform fluid density will simply be written ρ_f .

located at $\mathbf{x}_p$. The temperature and composition at the surface of the particle are noted T_p and $C_{\alpha,p}$, respectively. To realize the fluid-solid coupling, we impose the no-slip boundary condition and the continuity of the scalar fields, i.e.

$$\mathbf{u} = \mathbf{U}_p(\mathbf{X}) \quad (1.5a)$$

$$T = T_p(\mathbf{X}) \quad (1.5b)$$

$$C_\alpha = C_{\alpha,p}(\mathbf{X}), \text{ for } \alpha = 1, \dots, N_s, \quad (1.5c)$$

$$\forall \mathbf{X} \in \partial V_p.$$

Solid phase

The equations that govern the translational and rotational motion of a spherical particle are given by

$$m_p \frac{d\mathbf{u}_p}{dt} = \mathbf{F}_p + (\rho_s - \rho_{f0})V_p \mathbf{g} + \mathbf{F}_c \quad (1.6a)$$

$$I_p \frac{d\mathbf{\Omega}_p}{dt} = \mathbf{M}_p + \mathbf{M}_c \quad (1.6b)$$

$$\frac{d\mathbf{x}_p}{dt} = \mathbf{u}_p \quad (1.6c)$$

$$\frac{d\mathbf{q}_p}{dt} = \frac{1}{2} \mathbf{Q} \bar{\mathbf{Q}}_p, \quad (1.6d)$$

where ρ_s is the solid phase density, $m_p = \rho_s V_p$ is the mass of the particle, $I_p = \frac{1}{10} m_p d_p^2$ is the moment of inertia a sphere ($I_p = \frac{1}{8} m_p d_p^2$ for a disk in 2-D), $\mathbf{q}_p = (q_0, q_1, q_2, q_3)^T$ is the quaternion describing the orientation of the body in three dimensions, $\mathbf{F}_p$ and $\mathbf{M}_p$ correspond to the force and torque (or moment) exerted by the fluid on the particle while $\mathbf{F}_c$ and $\mathbf{M}_c$ are the resultant of the solid contact forces and torques, respectively. In a Cartesian frame, $\mathbf{Q}$ and $\bar{\mathbf{Q}}_p$ are expressed as

$$\mathbf{Q} = \begin{pmatrix} q_0 & -q_1 & -q_2 & -q_3 \\ q_1 & q_0 & -q_3 & q_2 \\ q_2 & q_3 & q_0 & -q_1 \\ q_3 & -q_2 & q_1 & q_0 \end{pmatrix} \quad \text{and} \quad \bar{\mathbf{Q}}_p = \begin{pmatrix} 0 \\ \Omega_{p,x} \\ \Omega_{p,y} \\ \Omega_{p,z} \end{pmatrix}. \quad (1.7)$$

The use of quaternions is justified by the well-known *gimbal lock* problem (singularity of the rotation matrix) that may appear when Euler angles are used to describe rotations in three dimensions [63].

The hydrodynamic force and torque at the surface of particle are given by

$$\mathbf{F}_p = \oint_{\partial V_p} \boldsymbol{\sigma} \cdot \mathbf{n} \, dS \quad (1.8a)$$

$$\mathbf{M}_p = \oint_{\partial V_p} \mathbf{r} \times (\boldsymbol{\sigma} \cdot \mathbf{n}) \, dS, \quad (1.8b)$$

where $\mathbf{n}$ is the outward unit normal vector at the surface of the particle and $\boldsymbol{\sigma}$ is the stress tensor. For a Newtonian fluid, $\boldsymbol{\sigma}$ is given by

$$\boldsymbol{\sigma} = \boldsymbol{\tau} - p\mathbf{I}, \quad (1.9)$$

with $\boldsymbol{\tau} = \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$, the viscous shear stress tensor and $\mathbf{I}$ the identity tensor.

When the temperature of the particle is allowed to evolve freely, the solid phase energy equation is given by

$$m_p c_{p,s} \frac{dT_p}{dt} = Q_p + Q_s, \quad (1.10)$$

where $c_{p,s}$ is the solid phase heat capacity, Q_p is the interfacial heat flux defined as

$$Q_p = \oint_{\partial V_p} k_f \nabla T \cdot \mathbf{n} \, dS \quad (1.11)$$

and Q_s is the heat source term in the solid phase. We also define the mass flux of species α at the surface of the particle as

$$J_{\alpha,p} = \oint_{\partial V_p} D_{\alpha,f} \nabla C_\alpha \cdot \mathbf{n} \, dS. \quad (1.12)$$

1.2.2 Immersed Boundary Method

Numerical method

The characteristic feature of the IBM is the use of two distinct grids, as illustrated in Figure 1.2. The fluid phase is solved on a Cartesian grid (here referred to as the Eulerian grid) with a uniform grid size h , while the surface of the particles is discretized using a set of Lagrangian points (here referred to as the Lagrangian grid). The present IBM has first been implemented in a self-developed 2-D Navier-Stokes solver and later in the in-house 3-D code *BigFlow*. The spatial operators are discretized using second- and fourth-order finite differences in the 2-D and 3-D solvers, respectively. The time-integration of Eqs. (1.3a) and (1.3b) is performed using a classic fractional-step scheme

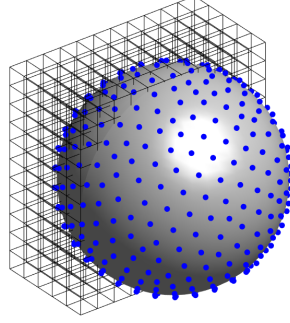


Figure 1.2: Eulerian grid of uniform mesh size h and distribution of the Lagrangian points over the surface of a spherical particle of diameter $d_p = 12h$.

on a staggered grid [70]. In a first step, the flow velocity is updated in the absence of any forcing (i.e. $\mathbf{f} = 0$). Then, the no-slip boundary condition at the surface of the solid bodies is enforced through the addition of the forcing term. Finally, a Poisson equation is solved for the pressure and the predictor velocity field is projected onto a divergent-free solution. The convective and diffusive terms are integrated with a constant time step Δt and using the Adams-Bashforth 2 and Euler schemes, respectively. The numerical scheme to advance the solution in the fluid phase from step n to step $n + 1$ thus reads

$$\mathbf{u}^* = \mathbf{u}^n + \Delta t \left(\left(\frac{3}{2} \mathbf{C}_{\mathbf{u}}^n - \frac{1}{2} \mathbf{C}_{\mathbf{u}}^{n-1} \right) + \nu \nabla^2 \mathbf{u}^n - \frac{1}{\rho_{f_0}} \nabla p^n + \mathbf{B}^n \right) \quad (1.13a)$$

$$\mathbf{u}^{**} = \mathbf{u}^* + \Delta t \mathbf{f} \quad (1.13b)$$

$$\nabla^2 \Phi = \rho_{f_0} \frac{\nabla \cdot \mathbf{u}^{**}}{\Delta t} \quad (1.13c)$$

$$\mathbf{u}^{n+1} = \mathbf{u}^{**} - \frac{\Delta t}{\rho_{f_0}} \nabla \Phi \quad (1.13d)$$

$$p^{n+1} = p^n + \Phi, \quad (1.13e)$$

where $\mathbf{C}_{\mathbf{u}} = -(\mathbf{u} \cdot \nabla) \mathbf{u}$, $\mathbf{u}^*$ and $\mathbf{u}^{**}$ are intermediate predictor velocity fields and Φ is the pressure correction.

In the numerical scheme given by Eqs. (1.13a)-(1.13e), it must be noted that the forcing is applied to the first predictor field $\mathbf{u}^*$ so that $\mathbf{u}^{**}$ verifies fairly well the boundary condition. Because of the velocity correction step, $\mathbf{u}^{n+1}$ will no longer exactly satisfy the no-slip boundary condition at the surface of the particle. Alternatively, one could first

impose the divergence-free constraint on $\mathbf{u}^{**}$ and apply the IBM forcing in a next step. In that case, the final velocity field $\mathbf{u}^{n+1}$ would better satisfy the boundary condition, but the continuity equation would not be exactly fulfilled. This is the approach considered in most studies based on the Discrete Lagrange Multiplier / Fictitious Domain (DLM/FD) method [50, 147]. To satisfy both the rigid-body motion and the incompressibility constraints at the end of the time step, we should enforce them together and not in a decoupled way. In our case, this would require an iterative procedure and solving multiple Poisson equations at each time step, hence increasing significantly the computational cost.

The scalar transport equations are integrated in a similar way after the flow has been updated:

$$T^* = T^n + \Delta t \left(\left(\frac{3}{2} C_T^n - \frac{1}{2} C_T^{n-1} \right) + \alpha_f \nabla^2 T^n + S_T^n \right) \quad (1.14a)$$

$$C_\alpha^* = C_\alpha^n + \Delta t \left(\left(\frac{3}{2} C_{C_\alpha}^n - \frac{1}{2} C_{C_\alpha}^{n-1} \right) + D_{\alpha,f} \nabla^2 C_\alpha^n + S_\alpha^n \right) \quad (1.14b)$$

$$T^{n+1} = T^* + \Delta t q \quad (1.14c)$$

$$C_\alpha^{n+1} = C_\alpha^* + \Delta t j_\alpha, \quad (1.14d)$$

where $C_T = -\mathbf{u} \cdot \nabla T$ and $C_{C_\alpha} = -\mathbf{u} \cdot \nabla C_\alpha$.

Forcing evaluation

We detail here the calculation of the momentum forcing term $\mathbf{f}$. The approach is straightforwardly extended to the scalar forcing terms q and j_α .

Interpolation-spreading operations allow to transfer quantities between the Lagrangian and the Eulerian grids. The interpolation kernels proposed in the literature can be classified in two types: high-order discrete δ -functions [141, 98] and bi- or tri-linear functions [56, 117]. In the present work, we use the regularization kernel proposed by Roma [106] (belonging to the first type):

$$\delta_h(x) = \frac{1}{h} \begin{cases} \frac{1}{6} \left(5 - 3 \frac{|x|}{h} - \sqrt{1 - 3 \left(1 - \frac{|x|}{h} \right)^2} \right), & 0.5 < \frac{|x|}{h} \leq 1.5 \\ \frac{1}{3} \left(1 + \sqrt{1 - 3 \left(\frac{|x|}{h} \right)^2} \right), & \frac{|x|}{h} \leq 0.5 \\ 0, & \text{otherwise.} \end{cases} \quad (1.15)$$

This kernel extends over 3 grid cells and constitutes a good compromise between the order of the interpolation procedure and the computational cost, as we want to avoid

larger stencils. The multi-dimensional interpolation kernel is obtained as the product of the one-dimensional delta functions, i.e.

$$\delta_h(\mathbf{x}) = \delta_h(x)\delta_h(y)\delta_h(z). \quad (1.16)$$

The computation of the forcing term $\mathbf{f}$ in Eq. (1.13b) can be summarized as follows, where capital letters indicate quantities evaluated on the Lagrangian points:

1. Interpolate the predictor velocity $\mathbf{u}^*$ from the Eulerian to the Lagrangian grid:

$$\mathbf{U}_l^*(\mathbf{X}_l) = \sum_{\mathbf{x}} \mathbf{u}^*(\mathbf{x})\delta_h(\mathbf{x} - \mathbf{X}_l)h^3, \quad (1.17)$$

where $\mathbf{X}_l$ is the position vector of the Lagrangian point identified by the index l .

2. Compute the Lagrangian forcing $\mathbf{F}_l$ using the interpolated velocity $\mathbf{U}_l^*$ and the boundary condition $\mathbf{U}_p$:

$$\mathbf{F}_l(\mathbf{X}_l) = \frac{\mathbf{U}_p(\mathbf{X}_l) - \mathbf{U}_l^*(\mathbf{X}_l)}{\Delta t}. \quad (1.18)$$

3. Spread the forcing from the Lagrangian to the Eulerian grid:

$$\mathbf{f}(\mathbf{x}) = \sum_l \mathbf{F}_l(\mathbf{X}_l)\delta_h(\mathbf{x} - \mathbf{X}_l)\Delta V_l, \quad (1.19)$$

where ΔV_l is the discrete volume associated to each Lagrangian point defined later (see Eq. (1.23)).

It must be noted that since Lagrangian points are only distributed at the surface of the particles (and not in their volume), the forcing term $\mathbf{f}$ will be non-zero in a restricted area on each side of the immersed boundary.

For the scalars, the Lagrangian forcing terms Q_l and $J_{\alpha,l}$ are similarly obtained as

$$Q_l(\mathbf{X}_l) = \frac{T_p - T_l^*(\mathbf{X}_l)}{\Delta t}, \quad (1.20)$$

$$J_{\alpha,l}(\mathbf{X}_l) = \frac{C_{\alpha,p} - C_{\alpha,l}^*(\mathbf{X}_l)}{\Delta t}. \quad (1.21)$$

where T_l^* and $C_{\alpha,l}^*$ are interpolated on the Lagrangian grid from T^* and C_α^* .

Retraction distance

It has been widely acknowledged in the literature [56, 157, 77] that the interpolation procedure artificially increases the hydrodynamic radius of the body when the Lagrangian points are located exactly on the surface of the particle, leading to an over-estimation of the drag force. As depicted in Figure 1.3, a remedy to this problem is to retract slightly the Lagrangian points from the particle surface by a distance r_d . While the interpolation-spreading operation is first-order accurate, Breugem [15] argues that second-order accuracy may be achieved by "properly" choosing this retraction distance. Based on convergence studies, the author suggests to use $r_d/h = 0.3$. The same value was earlier suggested by other authors [157, 56] and we will use this value in the present work, unless otherwise stated. Ideally, the retraction distance should be calibrated with the flow parameters and the grid resolution, as proposed by Tang et al. [124]. For an asymptotically fine grid, the value given to the retraction distance will no longer impact the final result as the porous shell created by the interpolation-spreading operation will shrink to zero thickness.

However, it must be recognized that this calibration procedure appears to be more of a cure for an intrinsic flaw in the numerical method, as pointed out in [148]. Since the goal of PR-DNS is to obtain high fidelity results from first principles and involving a minimum amount of empiricism, this additional parameter seems to be in contradiction with the spirit of the method. As a matter of fact, numerical methods that do not rely on a calibration of the hydrodynamic radius all use the information of the local outward normal vector, either to build asymmetric interpolation stencils in a DLM/FD framework [148] or to build mirror points on the other side of the interface such as in the PReIBM approach [132]. Moreover, the extension of this calibration procedure to non-spherical objects is not straightforward.

Building the Lagrangian grid

The number N_l of Lagrangian points distributed at the surface of a particle is chosen following the guidelines given in [15]:

1. the volume ΔV_l associated to each point is approximately equal to the volume of an Eulerian grid cell, i.e. $\Delta V_l \simeq h^3$,
2. the radial thickness of the porous shell that encompasses the Lagrangian grid is equal to h ,
3. N_l is an integer number.

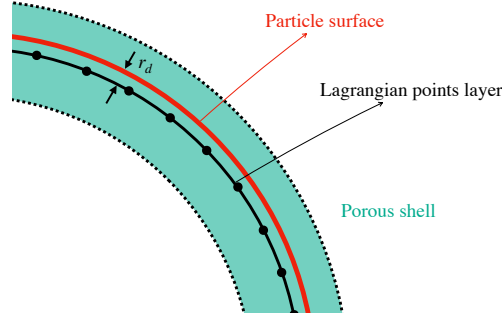


Figure 1.3: Retraction of the Lagrangian points layer by a distance r_d from the particle surface.

It follows that, in 3-D, N_l and ΔV_l are given by

$$N_l = \text{int} \left[\frac{\frac{4\pi}{3} ((R - r_d + h/2)^3 - (R - r_d - h/2)^3)}{h^3} \right], \quad (1.22)$$

and

$$\Delta V_l = \frac{\frac{4\pi}{3} ((R - r_d + h/2)^3 - (R - r_d - h/2)^3)}{N_l}. \quad (1.23)$$

The same kind of reasoning is used to determine N_l and ΔV_l in two-dimensional configurations. In 2-D, the even distribution of the Lagrangian points over the perimeter of a disk is straightforward. In 3-D, it is not possible to obtain a perfectly even distribution of a set of points over the surface of a sphere². To obtain the most regular grid possible, electric charges are given to the Lagrangian points and a separate simulation is run to solve a potential minimization problem [141]. Under the action of repulsive forces, Lagrangian points move over the surface of the sphere until an equilibrium is reached. It can then be considered that the points are almost uniformly distributed and their final position is used to build the grid.

Multidirect forcing

In the interpolation-spreading procedure described by Eqs. (1.17) to (1.19), Lagrangian points might *share* Eulerian grid points, so that they cannot be updated in-

²Except in a few particular cases: the Platonic solids.

dependently. Indeed, the forcing needed on one Lagrangian point will be impacted by how well the boundary condition is satisfied on its neighbor Lagrangian points and vice-versa. As a consequence, the condition $\mathbf{U}_l^* = \mathbf{U}_p(\mathbf{X}_l)$ may not be exactly satisfied after Eq. (1.13b). To better enforce the boundary condition, Luo et al. [76] proposed to add a multidirect forcing algorithm (MDF). The idea is to iterate on Eqs. (1.17) to (1.19) until the boundary condition is satisfied on all Lagrangian points with a given precision level. The iterative process is as follows:

Set: $\mathbf{u}^{*,0} = \mathbf{u}^*$ and $\mathbf{F}_l^{n,0} = 0$

for $k = 1 \rightarrow M$ **do**

$$\mathbf{U}_l^{*,k}(\mathbf{X}_l) = \sum_{\mathbf{x}} \mathbf{u}^{*,k-1}(\mathbf{x}) \delta_h(\mathbf{x} - \mathbf{X}_l) h^3 \quad (1.24a)$$

$$\mathbf{F}_l^{n,k}(\mathbf{X}_l) = \mathbf{F}_l^{n,k-1} + \frac{\mathbf{U}_p^n(\mathbf{X}_l) - \mathbf{U}_l^{*,k}(\mathbf{X}_l)}{\Delta t} \quad (1.24b)$$

$$\mathbf{f}^{n,k}(\mathbf{x}) = \sum_l \mathbf{F}_l^{n,k}(\mathbf{X}_l) \delta_h(\mathbf{x} - \mathbf{X}_l) \Delta V_l \quad (1.24c)$$

$$\mathbf{u}^{*,k} = \mathbf{u}^* + \Delta t \mathbf{f}^{n,k} \quad (1.24d)$$

end

where M is the number of forcing iterations. It must however be kept in mind that interpolation-spreading operations can be costly given the expression of the discrete δ -functions (Eq. (1.15)). To limit the computational overhead, M is therefore kept at a low value. In the present work, we use $M = 3$ as suggested in [15] and further supported by error analyses presented below.

1.2.3 Hydrodynamic forces and scalar fluxes

In Eqs. (1.8a) and (1.8b), $\mathbf{F}_p$ and $\mathbf{M}_p$ are expressed as surface integrals. More conveniently, they can be evaluated numerically by volume integration. Using the Green-Ostrogradski theorem and the expression of the fluid momentum balance given by Eq. (1.3b), the fluid force experienced by a particle can be expressed as

$$\begin{aligned} \mathbf{F}_p &= \oint_{\partial V_p} \boldsymbol{\sigma} \cdot \mathbf{n} \, dS = \int_{V_p} \nabla \cdot \boldsymbol{\sigma} \, dV \\ &= \rho_{f0} \left[- \int_{V_p} \mathbf{f} \, dV + \frac{d}{dt} \int_{V_p} \mathbf{u} \, dV - \int_{V_p} \mathbf{B} \, dV \right], \end{aligned} \quad (1.25)$$

where we identify the contributions of the IBM forcing term, the fluid inertia and the buoyancy term. The net torque exerted by the fluid on the particle can be similarly

expressed as

$$\begin{aligned}
 \mathbf{M}_p &= \oint_{\partial V_p} \mathbf{r} \times (\boldsymbol{\sigma} \cdot \mathbf{n}) \, dS = \int_{V_p} \mathbf{r} \times (\nabla \cdot \boldsymbol{\sigma}) \, dV \\
 &= \rho_{f_0} \left[\int_{V_p} \mathbf{r} \times \mathbf{f} \, dV + \frac{d}{dt} \int_{V_p} \mathbf{r} \times \mathbf{u} \, dV \right. \\
 &\quad \left. - \int_{V_p} \mathbf{r} \times \mathbf{B} \, dV \right]. \tag{1.26}
 \end{aligned}$$

If the Lagrangian points were located exactly on the surface of the spherical particle, about half of the $\mathbf{f}$ distribution would be located outside the volume of the particle. Therefore, simply summing all the non-zero values of $\mathbf{f}$ (including those outside the particle) would yield incorrect values of the force. Yet, Breugem [15] showed that by retracting the Lagrangian points from the surface, the contribution of the IBM forcing can be evaluated as

$$\rho_{f_0} \int_{V_p} \mathbf{f} \, dV \simeq \rho_{f_0} \sum_{\mathbf{x}} \mathbf{f}(\mathbf{x}) h^3. \tag{1.27}$$

In addition, thanks to the conservation properties of Roma's kernel functions, the summation can be performed on the Lagrangian grid, i.e.

$$\rho_{f_0} \sum_{\mathbf{x}} \mathbf{f}(\mathbf{x}) h^3 \simeq \rho_{f_0} \sum_{l=1}^{N_l} \mathbf{F}_l \Delta V_l. \tag{1.28}$$

Regarding the second term in the right-hand side (rhs) of Eq. 1.25, namely the fluid inertia contained within the volume occupied by the body, Uhlmann [141] makes the following approximation:

$$\frac{d}{dt} \left(\int_{V_p} \mathbf{u} \, dV \right) \simeq V_p \frac{d\mathbf{u}_p}{dt}, \tag{1.29}$$

which amounts to assume that the fluid inside the particle domain has a rigid-body motion. Although this assumption is fairly well verified in practice, it was pointed out by several authors [15, 43, 66] that it can lead to instabilities in the integration of Newton-Euler equations for low density ratio, i.e. when $\rho_r \triangleq \frac{\rho_s}{\rho_{f_0}}$ approaches unity. In his original work, Uhlmann [141] mentions a lower bound $\rho_r = 1.2$ before instabilities arise. This phenomenon is a direct consequence of the weak coupling of the fluid-structure interaction problem. As proposed by Breugem [15], we choose instead to explicitly account for the fluid inertia, which is numerically evaluated as

$$\int_{V_p} \mathbf{u} \, dV = \sum_{ijk} \chi_{s,ijk} \mathbf{u}_{ijk} h^3, \tag{1.30}$$

where χ_s is the solid phase indicator (or "mask") function. When χ_s is allowed to vary continuously between 0 (fluid phase) and 1 (solid phase), it can be considered as the fraction of the grid cell occupied by the solid. Kempe et al. [66] proposed to compute the solid fraction from a level set function as

$$\chi_{s,ijk} = \frac{\sum_{n=1}^8 -\phi_n H(-\phi_n)}{\sum_{n=1}^8 |\phi_n|}, \quad (1.31)$$

where ϕ is the signed distance to the interface ($\phi < 0$ inside and $\phi > 0$ outside the particle) and H is the Heaviside step function. The summation is performed over the eight corners of the grid cell (i, j, k) as illustrated in Figure 1.4.

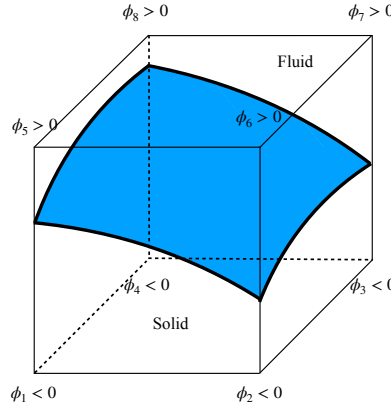


Figure 1.4: Calculation of the solid volume fraction at the center of a grid cell using the level set function at the eight corners (image inspired from [65]).

Finally, the hydrodynamic force and torque are numerically evaluated as

$$\mathbf{F}_p^n = \rho_{f_0} \left[- \sum_l \mathbf{F}_l^n \Delta V_l + \frac{1}{\Delta t} \left(\left\{ \int_{V_p} \mathbf{u} dV \right\}^{n+1} - \left\{ \int_{V_p} \mathbf{u} dV \right\}^n \right) - \int_{V_p} \mathbf{B}^n dV \right], \quad (1.32)$$

$$\begin{aligned} \mathbf{M}_p^n = \rho_{f_0} \left[- \sum_l (\mathbf{r}_l^n \wedge \mathbf{F}_l^n) \Delta V_l + \frac{1}{\Delta t} \left(\left\{ \int_{V_p} \mathbf{r} \wedge \mathbf{u} dV \right\}^{n+1} - \left\{ \int_{V_p} \mathbf{r} \wedge \mathbf{u} dV \right\}^n \right) \right. \\ \left. - \int_{V_p} (\mathbf{r}^n \wedge \mathbf{B}^n) dV \right]. \end{aligned} \quad (1.33)$$

With the same reasoning, the interfacial heat and mass fluxes can be easily computed as

$$\begin{aligned} Q_p = \rho_{f_0} c_{p,f} \left[- \int_{V_p} q dV + \frac{d}{dt} \int_{V_p} T dV \right] \\ \simeq \rho_{f_0} c_{p,f} \left[- \sum_l Q_l \Delta V_l + \frac{d}{dt} \int_{V_p} T dV \right] \end{aligned} \quad (1.34)$$

and

$$\begin{aligned} J_{\alpha,p} = - \int_{V_p} j_\alpha dV + \frac{d}{dt} \int_{V_p} C_\alpha dV \\ \simeq - \sum_l J_{\alpha,l} \Delta V_l + \frac{d}{dt} \int_{V_p} C_\alpha dV. \end{aligned} \quad (1.35)$$

1.2.4 Solid phase motion

The motion of the solid particles is advanced just after the flow has been updated by Eqs. (1.13a) to (1.13e) using a Discrete Element Method (DEM). To properly resolve the (potentially stiff) particle-particle and particle-wall contacts, and as proposed in [18], the time step Δt_s of the DEM solver is taken as a fraction of the time step used for the fluid solver, i.e. $\Delta t_s = \Delta t / n_{ss}$, where n_{ss} is the number of solid sub-steps per fluid time step. The fluid

forces are kept constant through the following sub-time stepping procedure:

Set: $\mathbf{u}_p^{k=0} = \mathbf{u}_p^n, \mathbf{\Omega}_p^{k=0} = \mathbf{\Omega}_p^n, \mathbf{x}_p^{k=0} = \mathbf{x}_p^n, \mathbf{q}_p^{k=0} = \mathbf{q}_p^n$

for $k = 1 \rightarrow n_{ss}$ **do**

$$\mathbf{u}_p^k = \mathbf{u}_p^{k-1} + \frac{\Delta t_s}{V_p \rho_s} \mathbf{F}_p^n + \frac{\Delta t_s}{V_p \rho_s} \frac{(\mathbf{F}_c^k + \mathbf{F}_c^{k-1})}{2} + \Delta t_s \frac{(\rho_s - \rho_{f0})}{\rho_s} \mathbf{g} \quad (1.36a)$$

$$\mathbf{\Omega}_p^k = \mathbf{\Omega}_p^{k-1} + \frac{\Delta t_s}{I_p} \mathbf{M}_p^n + \frac{\Delta t_s}{I_p} \frac{(\mathbf{M}_c^k + \mathbf{M}_c^{k-1})}{2} \quad (1.36b)$$

$$\mathbf{x}_p^k = \mathbf{x}_p^{k-1} + \frac{\Delta t_s}{2} (\mathbf{u}_p^k + \mathbf{u}_p^{k-1}) \quad (1.36c)$$

$$\mathbf{q}_p^k = \mathbf{q}_p^{k-1} + \frac{\Delta t_s}{2} \left(\frac{1}{2} \mathbf{Q}^k \mathbf{\Omega}_p^k + \frac{1}{2} \mathbf{Q}^{k-1} \mathbf{\Omega}_p^{k-1} \right) \quad (1.36d)$$

end

Set: $\mathbf{u}_p^{n+1} = \mathbf{u}_p^{k=n_{ss}}, \mathbf{\Omega}_p^{n+1} = \mathbf{\Omega}_p^{k=n_{ss}}, \mathbf{x}_p^{n+1} = \mathbf{x}_p^{k=n_{ss}}, \mathbf{q}_p^{n+1} = \mathbf{q}_p^{k=n_{ss}}.$

Unless otherwise stated, $n_{ss} = 20$ granular sub-time steps are performed per fluid time step. The Crank-Nicolson scheme used to integrate the collision part requires the knowledge of $\mathbf{F}_c^k$ and $\mathbf{M}_c^k$, i.e. the contact terms at the end of the sub-time step. Practically, $\mathbf{F}_c^k$ and $\mathbf{M}_c^k$ are iteratively computed as a function of the new particle position until the distance between two consecutive estimates of $\mathbf{x}_p^k$ is below a chosen tolerance ϵ (i.e. $\Delta \mathbf{x}_p \triangleq \|\mathbf{x}_p^{k,\text{new}} - \mathbf{x}_p^{k,\text{old}}\| < \epsilon$). For most simulations presented in this work, only two passes in the loop are sufficient to satisfy $\Delta \mathbf{x}_p < 1 \times 10^{-5} h$. To calculate the contact forces, a combined soft-sphere/lubrication model is employed as proposed in [18]. The details of the model and the parameters used are given in Appendix A.

Finally, the velocity of the Lagrangian points at the surface of the particles is updated as

$$\mathbf{U}_{p,l}(\mathbf{X}_l^{n+1}) = \mathbf{u}_p^{n+1} + \mathbf{\Omega}_p^{n+1} \wedge \mathbf{r}_l \quad (1.37)$$

Due to the rigidity assumption, the position vector $\mathbf{r}_l = \mathbf{X}_l - \mathbf{x}_p$ expressed in a body-fixed frame does not vary in time.

1.3 Definitions

We introduce in this section a number of quantities that will be used repeatedly in this document to characterize a problem or to report results.

The particle Reynolds number is defined as

$$\text{Re}_p = \frac{U_0 d_p}{\nu}, \quad (1.38)$$

where U_0 is a reference velocity. The choice of U_0 is context-dependent. For cases with open boundaries with an inflow velocity U_∞ , it will be the natural choice for U_0 . In closed (or semi-closed) domains, the motion of the flow will be typically driven by gravity. A particle in free-fall reaches its terminal velocity U_t when the drag and the buoyancy forces balance each other, i.e.

$$V_p(\rho_s - \rho_{f_0})g = \frac{1}{2}\rho_{f_0}U_t^2 C_d A_p, \quad (1.39)$$

where C_d is the drag coefficient acting on the particle and A_p is the projected surface area. Namely, $V_p = \frac{\pi d_p^3}{6}$ and $A_p = \frac{\pi d_p^2}{4}$ for a sphere in 3-D while $V_p = \frac{\pi d_p^2}{4}$ and $A_p = d_p$ for a cylinder in 2-D. By analogy, the characteristic velocity U_c for sedimentation problems is defined by stating that

$$V_p(\rho_s - \rho_{f_0})g = \frac{1}{2}\rho_{f_0}U_c^2 A_p. \quad (1.40)$$

Hence, U_c is given by

$$U_c = \sqrt{\frac{\pi d_p}{2}(\rho_r - 1)g} \quad \text{in 2-D}, \quad (1.41)$$

and

$$U_c = \sqrt{\frac{4d_p}{3}(\rho_r - 1)g} \quad \text{in 3-D}. \quad (1.42)$$

We deduce from Eqs. (1.39) and (1.40) that the drag coefficient when the particle has reached its terminal velocity can be expressed as

$$C_d = \frac{U_c^2}{U_t^2}. \quad (1.43)$$

We also define the terminal Reynolds number as

$$Re_t = \frac{U_t d_p}{\nu}, \quad (1.44)$$

although U_t is usually not known a priori and is rather a result of the simulation.

Regarding heat and mass transfer, the Prandtl and Schmidt numbers are respectively defined as

$$Pr = \frac{\nu}{\alpha_f} \quad (1.45)$$

and

$$Sc_\alpha = \frac{\nu}{D_{\alpha,f}}, \quad (1.46)$$

for a specific species α .

Finally, the ratio between buoyancy and viscous forces is quantified by the Grashof number:

$$\text{Gr} = \frac{g\beta\Delta T d_p^3}{\nu^2}, \quad (1.47)$$

where ΔT is the characteristic temperature difference of the problem.

1.4 2-D validation test cases

1.4.1 Flow past a fixed cylinder

We first consider the flow past a fixed cylinder in a channel with a velocity U_∞ at the inflow. The domain has a size $30d_p \times 20d_p$ and the cylinder is located vertically in the middle of the domain and horizontally at a distance $10d_p$ from the inflow. In the transverse direction, we impose slip boundary conditions on the domain boundaries to minimize confinement effects. Figures 1.5a and 1.5b show the vorticity iso-contours for the cases at $\text{Re}_p = 40$ and $\text{Re}_p = 100$ with resolutions $N_d = \frac{d_p}{h} = 32$ and $N_d = 48$, respectively. At $\text{Re}_p = 100$, the flow is unsteady and the wake is characterized by von-Karman vortices.

The drag and lift coefficients of this flow are respectively defined as

$$C_d = \frac{F_{p,x}}{\frac{1}{2}\rho_{f0}U_\infty^2 d_p} \quad (1.48)$$

and

$$C_l = \frac{F_{p,y}}{\frac{1}{2}\rho_{f0}U_\infty^2 d_p}. \quad (1.49)$$

At $\text{Re}_p = 100$, we also define the Strouhal number $St = \frac{f_l U_\infty}{d_p}$, where f_l is the oscillation frequency of the lift coefficient. Our results for the time-averaged drag coefficient $\bar{C}_d$, the oscillation amplitude of the lift coefficient ΔC_l ³ and the Strouhal number are reported in Table 1.1. The comparison between our results using a retraction distance $r_d = 0.3h$ and the values given in the literature is quite satisfactory, although the drag coefficient is overestimated by a few percents in both cases, probably due to the slight confinements effects induced by the side walls. To illustrate the impact of the retraction distance r_d on the IBM results, the flow at $\text{Re}_p = 100$ is also computed using $r_d = 0$ and the same resolution $N_d = 48$. The time-averaged drag coefficient reported

³Here defined as half the peak-to-peak distance

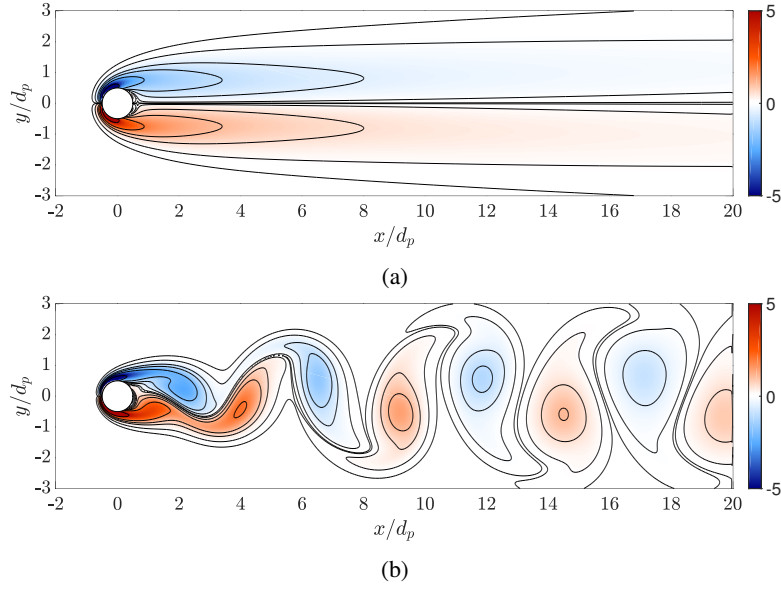


Figure 1.5: Vorticity iso-contours $\frac{\omega_z d_p}{U_0}$ of the flow past a fixed cylinder at (a) $Re_p = 40$ and (b) $Re_p = 100$.

in Table 1.1 is significantly larger, which confirms the substantial overestimation of the drag force when the Lagrangian points are not retracted from the particle surface. The same observation is made on the oscillation amplitude of the lift coefficient, while the Strouhal number is little affected by a change in the value given to r_d .

	$\bar{C}_d$	ΔC_l	St
$Re_p = 40$			
Present ($r_d = 0.3h$)	1.58	-	-
Canuto and Taira [16]	1.54	-	-
Apte et al. [6]	1.53	-	-
$Re_p = 100$			
Present ($r_d = 0.3h$)	1.38	0.333	0.170
Present ($r_d = 0$)	1.40	0.348	0.169
Canuto and Taira [16]	1.34	0.329	0.167
Mittal et al. [86]	1.35	-	0.165
Apte et al. [6]	1.36	-	0.165

Table 1.1: Flow past a fixed cylinder at $Re_p = 40$ and $Re_p = 100$: time-averaged drag coefficient, lift oscillation amplitude and Strouhal number.

To assess the convergence properties of the IBM, the case at $\text{Re}_p = 100$ has been simulated with different resolutions $N_d = (16, 20, 24, 32, 40, 48, 56)$. The value of the mean drag coefficient at "infinite" resolution $\bar{C}_{d_\infty}$ and the order of convergence p can be evaluated using Richardson's extrapolation [105]:

$$X_h = X_\infty + Ch^p, \quad (1.50)$$

where X_h is the solution obtained for a quantity X using a finite grid size h , X_∞ is the "exact" solution (i.e. that obtained with infinite resolution) and C is a constant. The convergence order p can then be found as the solution of

$$\frac{X_1 - X_2}{X_2 - X_3} = \frac{h_1^p - h_2^p}{h_2^p - h_3^p}, \quad (1.51)$$

where X_1 , X_2 and X_3 are the results obtained with grid sizes h_1 , h_2 and h_3 , respectively. Using the results of the three finest resolutions to evaluate $\bar{C}_{d_\infty}$, we show in Figure 1.6 the evolution of the relative error as the grid is refined. The order of convergence extracted from Eq. (1.51) is $p = 1.83$, i.e. a sub-quadratic convergence, yet much better than a first order convergence.

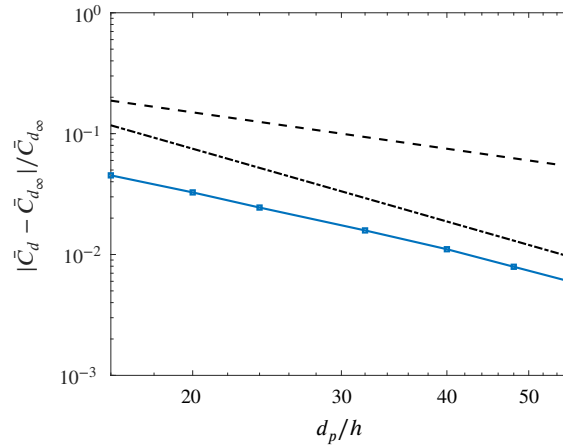


Figure 1.6: Spatial convergence of the error made on the mean drag coefficient at $\text{Re}_p = 100$ relatively to the value extrapolated at infinite resolution ($\blacksquare$). The first (- -) and second (- · -) order convergence lines are also shown for comparison.

1.4.2 Drafting-kissing-tumbling of two circular particles

Two circular particles of equal size are placed above each other in a cavity and accelerate from rest under the action of gravity. While falling, the wake induced by the bottom (or leading) particle will reduce the flow resistance faced by the top (or trailing) particle. As a result, the trailing particle will fall faster than the leading one and will eventually catch it. The two particles will momentarily form a pseudo single body. As this flow configuration is unstable, the two particles will tumble and finally split. This well-known phenomenon is called "drafting-kissing-tumbling" (DKT) and has been extensively studied in previous works [51, 96, 141]. For comparison purpose, we take the same reference velocity and length scales as Glowinski et al. [51] although they differ from our usual choices described in Section 1.3. The computational domain has dimensions $[0, 2l_0] \times [0, 6l_0]$, with $l_0 = 4d_p$, the reference length scale. The two particles are initially positioned at $(1, 4.5)l_0$ and $(1, 5)l_0$. The gravitational acceleration is $\mathbf{g} = -981(U_0^2/l_0)\mathbf{e}_y$, $\nu = 0.01(U_0 l_0)$ and the density ratio between the solid and the fluid is $\rho_r = 1.5$. The reference time scale is defined as $t_0 = \frac{l_0}{U_0}$. We used a resolution $N_d = 72$ and the time step is $\Delta t = 5 \times 10^{-6} t_0$.

Figure 1.7 shows vorticity iso-contours of this flow at different dimensionless times. The different stages of the DKT are well reproduced. We report in Figure 1.8 the evolution of the vertical position and velocity of the two falling particles in comparison to the reference results from Glowinski et al. [51]. In the "drafting" zone, the comparison is very good as the trajectories of the two particles coincide with the reference curves. Because the "tumbling" is triggered by a strong instability (viz. the "kissing" part) and that the results from [51] were obtained using a different numerical method (Discrete Lagrange Multiplier method in a finite-element framework), we can hardly expect more than a qualitative agreement after the touching of the two particles. The shapes of the curve are however very similar.

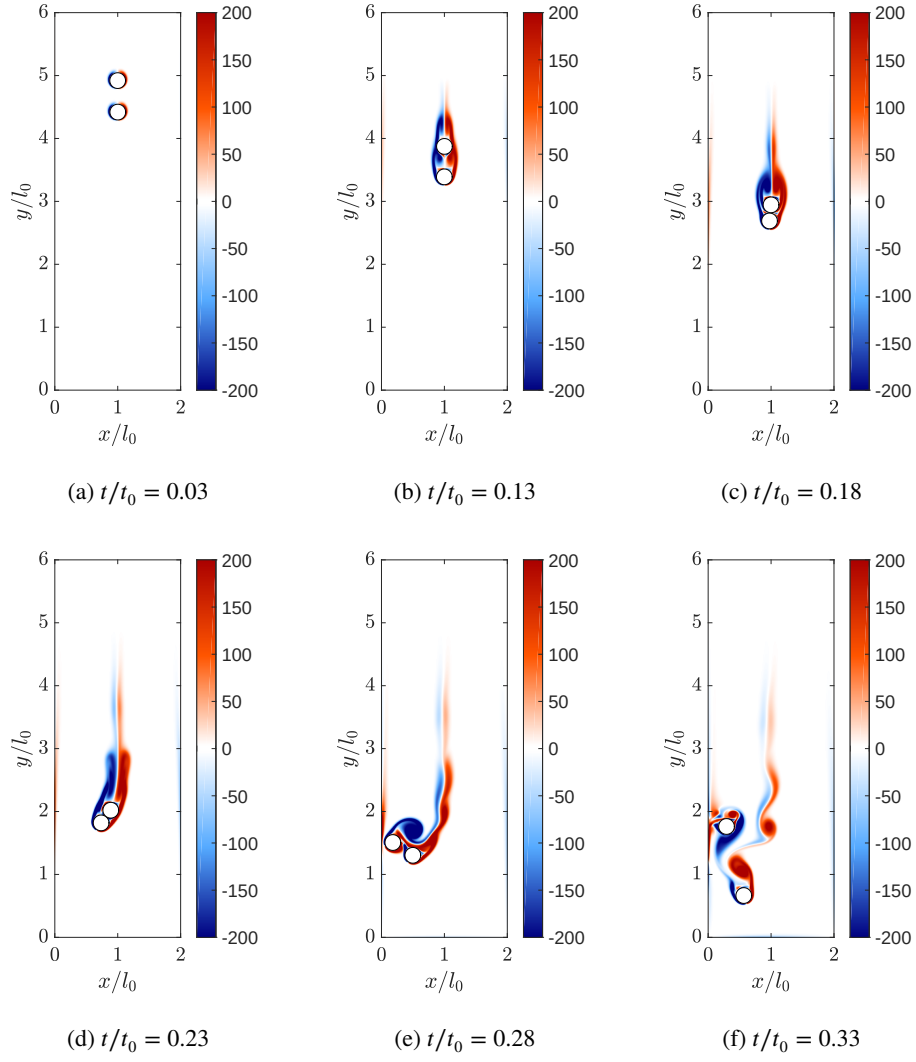
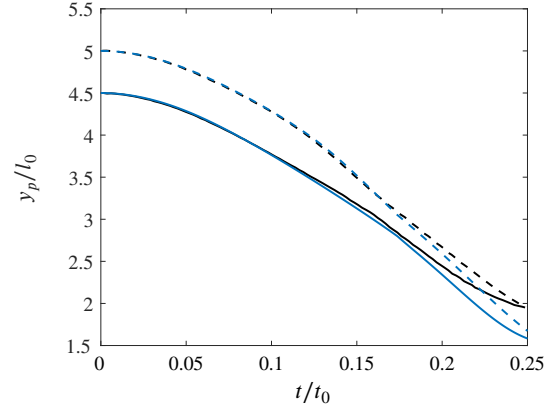
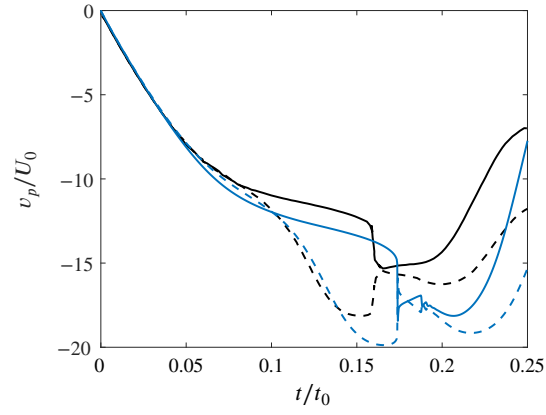


Figure 1.7: Vorticity iso-contours $\frac{\omega_z l_0}{U_0}$ at different stages of the drafting-kissing-tumbling of two cylinders in a cavity.



(a)



(b)

Figure 1.8: Drafting-kissing-tumbling of two cylindrical particles: time evolution of (a) the vertical position and (b) the velocity of the leading (solid line) and trailing (dashed line) particle. Present results (—) are compared to reference data from Glowinski (—) [51].

1.4.3 Sedimentation of a cold cylinder in a semi-infinite channel

As a first non-isothermal validation test case, we consider the problem of a cold cylinder falling in a semi-infinite hot channel at different Grashof numbers. This problem was previously studied by Gan et al. [46], Yu et al. [158] and Wachs [147], among others. The particle has a constant temperature T_p while the fluid temperature is initialized to the temperature of the side walls, T_0 , so that $\Delta T = T_0 - T_p > 0$.

The computational domain has a size $4d_p \times 32d_p$ and the center of the particle is initially located at $1.5d_p$ from the left wall and $8d_p$ from the top boundary. To mimic a semi-infinite channel in the vertical direction, we use the same technique as other authors by shifting the solution upwards once the cylinder falls below a distance $8d_p$ from the bottom boundary. The density ratio is $\rho_r = 1.00232$, the Prandtl number is $Pr = 0.7$ and the particle Reynolds number based on the characteristic velocity defined by Eq. (1.41) is $Re_p = 40.5$. The Gr number varies from 0 to 5000 to highlight the different sedimentation regimes identified in previous studies [46, 158, 147]:

- Regime A, $0 < Gr < 500$: steady settling of the particle along the centerline, symmetric wake vortices,
- Regime B, $500 < Gr < 810$: vortex shedding and low amplitude oscillations of the particle along the centerline,
- Regime C, $810 < Gr < 2150$: steady settling of the particle close to one of the walls, no vortex shedding,
- Regime A', $2150 < Gr < 3500$: steady settling of the particle along the centerline, symmetric wake vortices,
- Regime B', $3500 < Gr < 4300$: vortex shedding and low amplitude oscillations of the particle along the centerline,
- Regime D, $Gr > 4300$: turbulent-like wake vortices and large amplitude oscillations of the particle along the centerline.

As mentioned in [147], the transition values 3500 and 4300 are only indicative bounds of the transition regime between the steady settling (A') and the strongly oscillatory (D) regimes, whose onset can be triggered by small instabilities in the flow.

All simulations have been performed with a resolution $N_d = 24$ and a time step $\frac{\Delta t U_c}{d_p} = 2 \times 10^{-3}$. Figure 1.9 shows the temperature field and the vorticity iso-contours to visualize the flow patterns at different Grashof numbers. The time evolution of the lateral position of the cylinder presented in Figure 1.10 confirms that our method is

able to reproduce the different sedimentation regimes when the Grashof number varies. While Yu et al. [158] detect the strongly unstable regime D at $Gr = 4500$, we still observe a periodic vortex shedding along the centerline at this Grashof number, like Gan et al. [46] as well as Wachs [147]. The regime D is well observed at $Gr = 5000$; the particle exhibits a strong oscillatory motion but it never touches the wall. Finally, Figure 1.11 compares the evolution of the terminal Reynolds number $Re_t = \frac{U_t d_p}{\nu}$ with Gr to the results of Yu et al. [158] and Wachs [147]. The agreement is very satisfactory, with the largest difference (3.5%) observed for $Gr = 5000$. It must also be noted that this test case confirms the ability of our method to handle particle flows with a low solid-fluid density ratio.

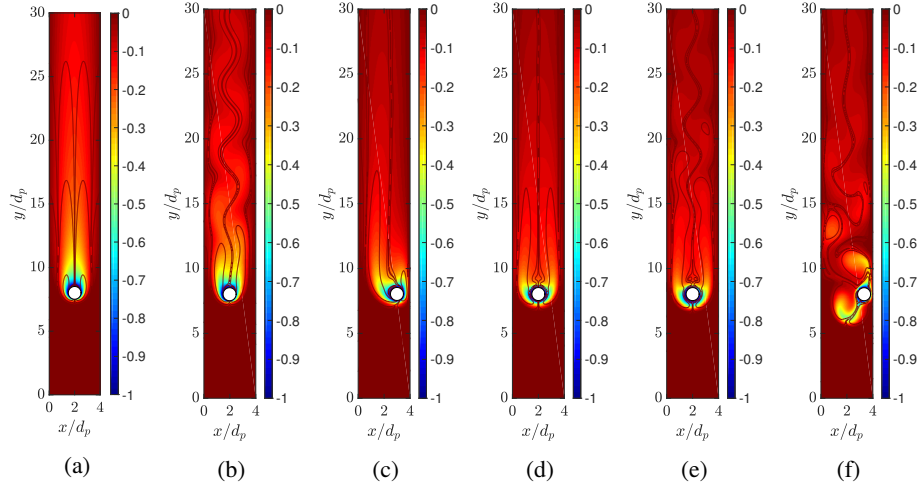


Figure 1.9: Temperature field $(T - T_0)/(T_0 - T_p)$ and vorticity iso-contours for a cold particle sedimenting in a narrow semi-infinite channel, at (a) $Gr = 0$, (b) $Gr = 564$, (c) $Gr = 1500$, (d) $Gr = 3000$, (e) $Gr = 4500$ and (f) $Gr = 5000$.

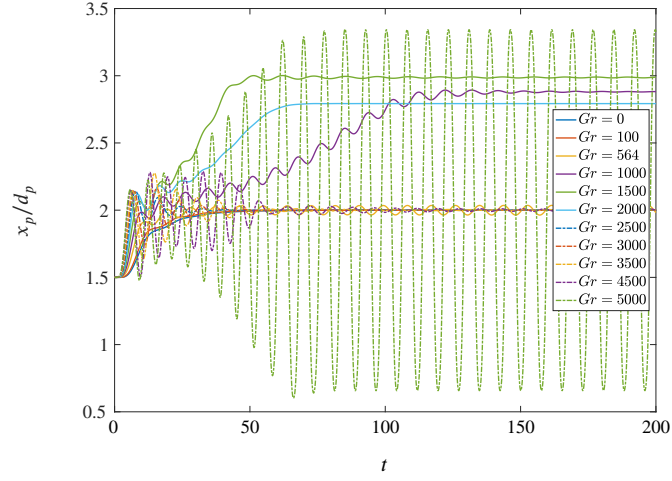


Figure 1.10: Time evolution of the lateral position of a cold cylinder sedimenting in a semi-infinite channel at different Grashof numbers.

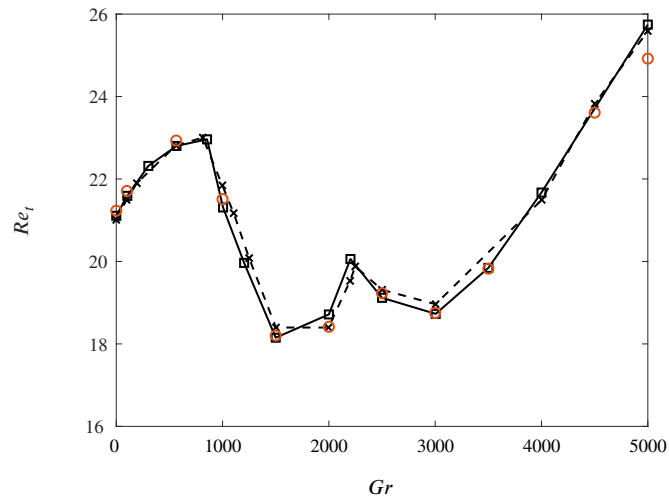
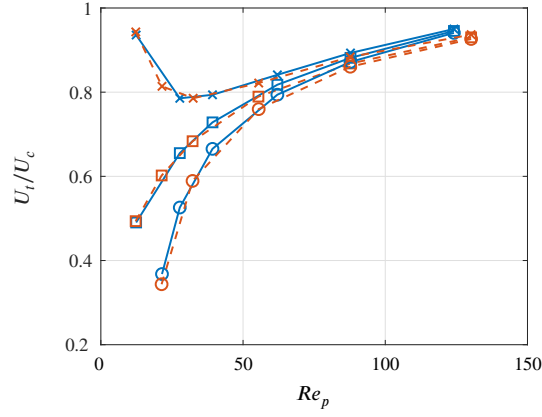


Figure 1.11: Terminal Reynolds number of a cold particle sedimenting in a semi-infinite channel as a function of the Grashof number: present results ($\circ$) compared to Wachs [147] ($-x-$) and Yu et al. [158] ($- \blacksquare -$).

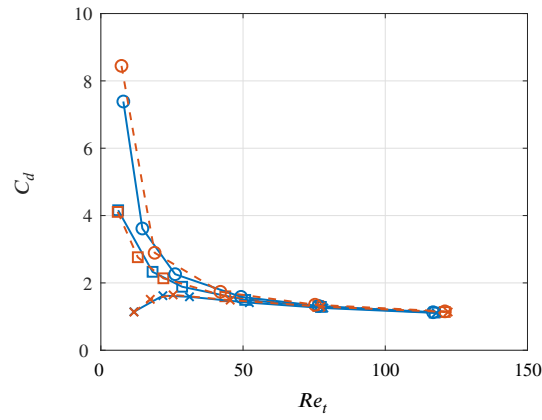
1.4.4 Sedimentation of a buoyant cylinder in an enclosure

To further validate the accuracy of our method, we now study the sedimentation of a buoyant cylinder in an enclosure for increasing values of ρ_r and at three different Grashof numbers: 0, 100 (cylinder hotter than the fluid) and -100 (cylinder cooler than the fluid). This problem was previously addressed by Feng et al. [44] and Wachs [147]. The reference velocity is still defined by Eq. (1.41). The density ratio varies between 1.001 and 1.1 and the corresponding particle Reynolds number is in the range [12.4, 124]. The Prandtl number is $Pr = 1$. The enclosure has a size $16d_p \times 40d_p$ and the resolution is $N_d = 16$.

The terminal velocity of the particle and the drag coefficient given by Eq. (1.43) are reported in Figure 1.12 as a function of Re_p and Re_t , respectively, and for the three Grashof numbers. When the particle is hotter than the fluid, the natural convection effects act in the opposite direction to gravity, slowing down the particle as it falls. The drag coefficient is therefore larger at $Gr = 100$ compared to $Gr = 0$. At $Gr = -100$, the reverse phenomenon happens: the natural convection effects and gravity act in the same direction and the settling velocity of the particle increases. At high Reynolds number (i.e. high density ratio), the natural convection effects become negligible in front of the particle weight and the terminal velocity is independent of Gr . The comparison between our results and those reported by Wachs [147] is very satisfactory although slight deviations can be observed in Figure 1.12a for the terminal velocity at high Re_p . These small differences are attributed to the relatively coarse resolution we used and the higher sensitivity of the solution to the value given to the retraction distance (here $r_d = 0.3h$) at high Reynolds number. At low Re_p , our results and those of Wachs [147] are very similar, while those reported by Feng et al. [43] (not shown here) indicate stronger natural convection effects, with lower (higher) terminal velocities at $Gr = 100$ (-100). We think this difference might be due to the fact that Feng et al. do not seem to include the integral buoyancy term in the expression of the hydrodynamic force (i.e. the third term on the right-hand side of Eq. (1.25)).



(a)



(b)

Figure 1.12: Sedimentation of a cylinder in an enclosure at $Gr = 0$ ($\square$), $Gr = 100$ ($\circ$) and $Gr = -100$ ($\times$). Our results are compared to those reported by Wachs [147] (respectively $-\square-$, $-\circ-$ and $-\times-$): (a) terminal velocity vs. Re_p and (b) drag coefficient vs. Re_t .

1.4.5 Motion of a circular catalyst in an enclosure

As a last 2-D validation test, we consider the motion of a circular catalyst with freely evolving temperature in an enclosure. This test case was first examined by Yu et al. [158] and then by Feng and Michaelides [43] and Wachs [147]. The temperature of the particle is the result of the balance between the heat source term resulting from the reaction in the solid phase and the interfacial heat flux with the surrounding fluid (see Eq. (1.10)). The heat source term per unit volume in the solid phase is noted $q_s = \frac{Q_s}{V_p}$. In [158], Yu et al. solve the heat conduction problem inside the solid phase with a conductivity ratio $k_r = \frac{k_s}{k_f} = 15$, k_s being the solid phase conductivity. Instead, Wachs [147] uses a uniform solid phase temperature which amounts to take a very large (theoretically infinite) value for k_r . This latter approach is also adopted here. The dimensionless parameters of the problem are $\rho_r = 1.1$, $\text{Re}_p = 40$, $\text{Pr} = 0.7$, $\text{Gr} = 1000$ and $q_s^* = 1$, where $q_s^* = \frac{q_s d_p}{\rho_{f0} c_{p,f} U_c \Delta T}$ is the dimensionless heat source term per unit volume in the solid phase and ΔT is a chosen temperature scale. The heat capacity ratio $c_{p,r} = \frac{c_{p,f}}{c_{p,s}}$ varies from 0.2 to 5. The cavity has a size $8d_p \times 16d_p$ and the catalyst is initially located in the middle of the domain. The particle and the surrounding fluid are initially at the walls temperature T_0 . The resolution is $N_d = 24$ and the time step is $\frac{\Delta t U_c}{d_p} = 2 \times 10^{-3}$.

Figure 1.13 shows the temperature iso-contours at different dimensionless times $t^* = \frac{t U_c}{d_p}$ for the case at $c_{p,r} = 1$. The thermo-mechanical phenomenon that governs the catalyst motion can be succinctly described as follows. Initially, the vertical velocity of the particle takes negative values because the gravitational force is dominant. As the heat source term gradually increases the catalyst temperature, the fluid surrounding the particle is heated up and natural convection effects start prevailing over gravity. The catalyst rises in the enclosure, without colliding with the upper wall and eventually reaches an equilibrium position below the top of the domain when buoyancy and hydrodynamic forces balance each other.

We plot in Figure 1.14 the evolution of the catalyst vertical velocity as a function of time and for different $c_{p,r}$ values. In all cases, the particle exhibits the kind of motion described above. The comparison of our results with those reported by Wachs [147] is very good, although we obtain slightly larger values for the maximal velocity of the particle.

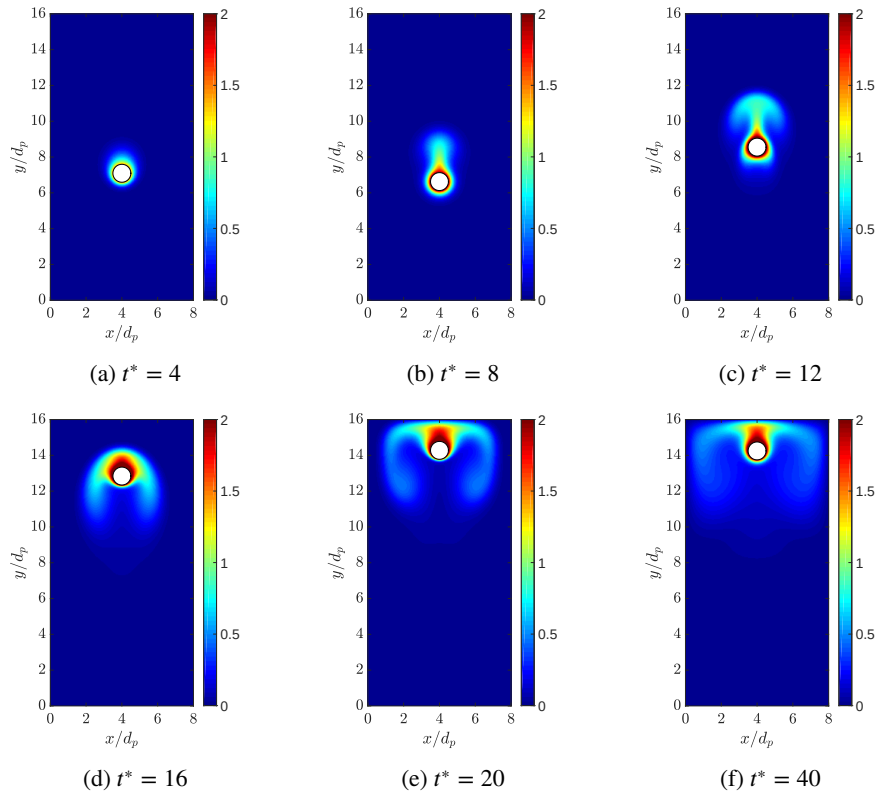


Figure 1.13: Motion of a circular catalyst in an enclosure: time evolution of the dimensionless temperature field $(T - T_0)/\Delta T$ with $\rho_r = 1.1$, $\text{Re}_p = 40$, $\text{Pr} = 0.7$, $\text{Gr} = 1000$, $q_s^* = 1$, $c_{p,r} = 1$.

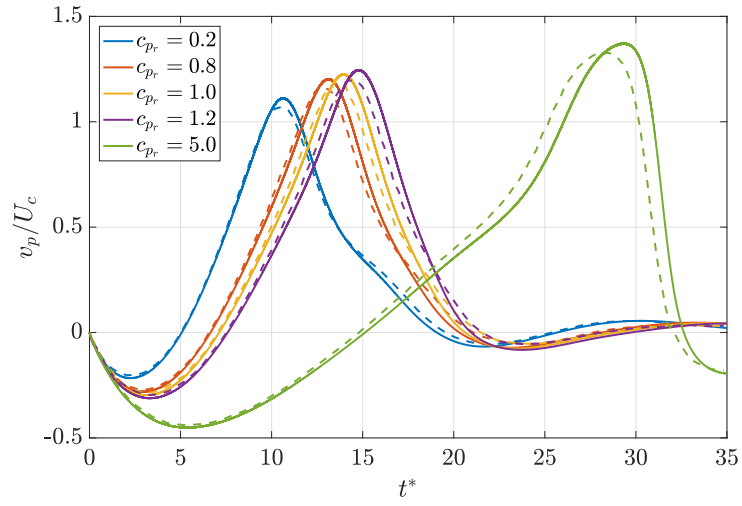


Figure 1.14: Vertical velocity component of a circular catalyst with varying temperature in an enclosure; $\rho_r = 1.1$, $\text{Re}_p = 40$, $\text{Pr} = 0.7$, $\text{Gr} = 1000$, $q_s^* = 1$. Present results (solid line) are compared with those reported by Wachs et al. [147] (dashed line).

1.5 3-D validation test cases

We now validate the implementation of the numerical method in the fourth-order finite-difference code *BigFlow* used for 3-D flows. The different features of the methodology are verified, namely: the accuracy of the boundary condition enforcement, the fluid-structure interaction, the extension of the IBM to heat and mass transfer and the coupling with natural convection effects.

1.5.1 Flow past a sphere at $\text{Re}_p = 300$

The flow past a sphere at $\text{Re}_p = \frac{U_\infty d_p}{\nu} = 300$ is a standard benchmark to verify numerical methods involving immersed bodies and it has been extensively used in literature as a validation tool ([100, 84, 116]). The computational domain has dimensions $[-3, 15]d_p \times [-4, 4]d_p \times [-4, 4]d_p$ and the sphere is located at the origin. The grid is stretched along the streamwise (x) direction to capture several periods of the wake structures while limiting the computational overhead⁴. The resolution is $N_d = 64$. As in [100, 116], a perturbation is introduced on the vertical component of the inflow to break the axisymmetry of the flow and trigger the wake instability. At the inflow, the velocity is thus given by $\mathbf{u}_\infty = U_\infty \mathbf{e}_x + V_\infty \mathbf{e}_y$, with

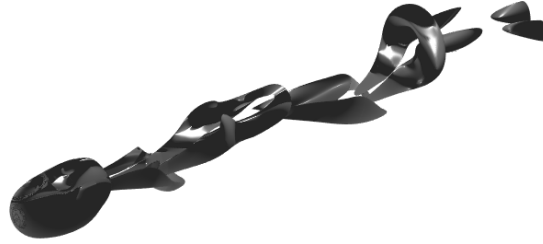
$$V_\infty = \begin{cases} 0.1 \sin(\pi(t^* - 3))U_\infty & \text{if } 3 < t^* < 4, \\ 0 & \text{otherwise.} \end{cases} \quad (1.52)$$

and $t^* = \frac{tU_\infty}{d_p}$. Natural outflow boundary conditions are used at $x = 15d_p$. Free-slip boundary conditions are imposed in the transverse (y and z) directions.

Figure 1.15 shows the periodic ring-shaped structures developed in the wake of the sphere. The perturbation added at the inflow breaks the symmetry in the xy plane while the wake is still symmetric in the xz plane, i.e. when viewed from above as in Figure 1.15b.

Since the flow is periodic, we compare in Figure 1.16 the vorticity iso-contours in the xy plane at each quarter period to the results obtained by Ploumhans et al. with their body-fitted vortex method [100]. The qualitative agreement seems very good. Finally, Figure 1.17 shows the time evolution of the drag and lift coefficients obtained with our method and the time-averaged values are compared to references from the literature. With a retraction distance $r_d/h = 0.3$, we obtain a mean value $\bar{C}_d = 0.693$, close to the results reported by Mimeau et al. [84] (0.673) and Ploumhans et al. [100]

⁴However, the grid size is fixed to a constant value in a defined area around the particle since the IBM is designed for a uniform grid.



(a) Side view.



(b) Top view.

Figure 1.15: Visualization of the vortical structures induced by the flow past a sphere at $Re_p = 300$ (iso-surface $\lambda_2 = -0.01$).

(0.683), although slightly larger. Satisfactorily, our prediction for the time-averaged lift coefficient ($\bar{C}_l = 0.064$) is comprised between those of Mimeau et al. [84] (0.066) and Ploumhans et al. [100] (0.061).

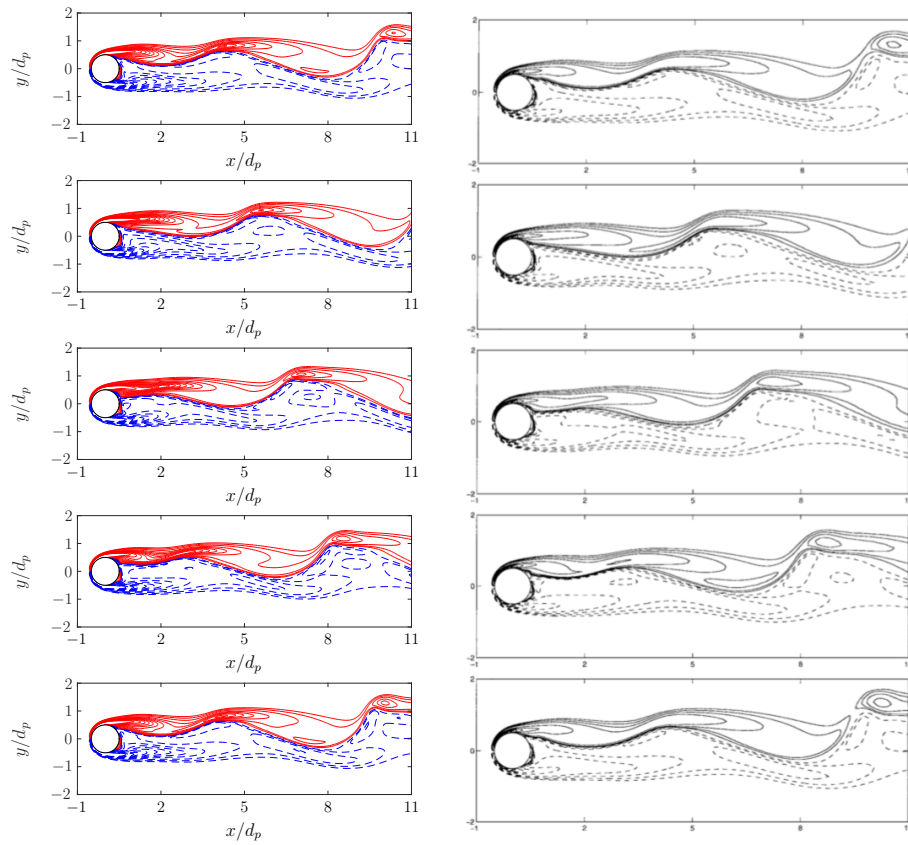
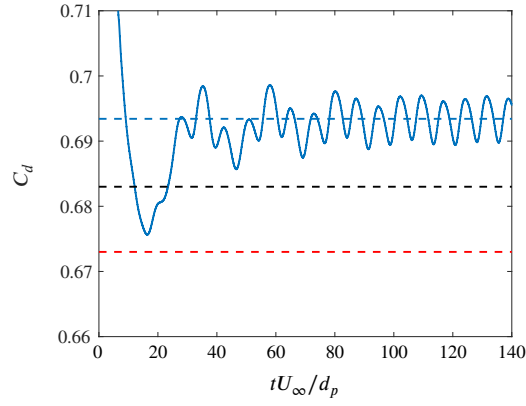
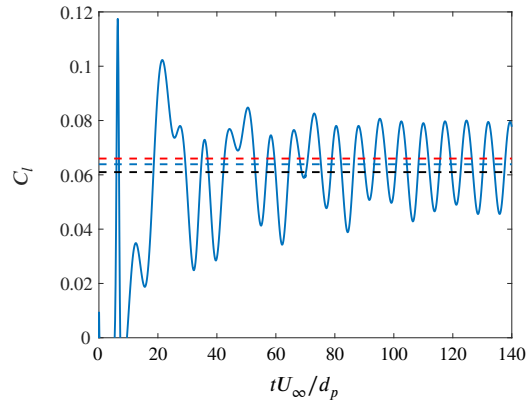


Figure 1.16: Flow past a sphere at $Re_p = 300$: iso-contours of $\frac{\omega_z d_p}{U_\infty}$ in the xy plane ($z = 0$) for each quarter period. Comparison between the present results (left) and those of Ploumhans et al. [100] (right). The contour levels range from -5 to 5 (excluding zero) with an increment of 0.5 and additional contours were drawn at ± 0.25 .



(a) Drag



(b) Lift

Figure 1.17: Flow past a sphere at $Re_p = 300$. Time evolution of (a) the drag and (b) the lift coefficients (—). Dashed lines correspond to time-averaged values when the flow is developed: comparison between the present results (—), those of Mimeau et al [84] (—) and Ploumhans et al. [100] (—).

1.5.2 Stokes flow past a periodic array of spheres

Very few particle flows can be solved analytically. Among them, we consider the flow past a periodic array of spheres in Stokes regime. A single sphere is placed at the center of a periodic cubic domain of dimension L to reproduce a simple cubic (SC) network. The flow rate (or superficial) velocity U_0 is prescribed by an external pressure gradient along the z direction. The solid volume fraction of the array is given by $\phi_s = \frac{\pi d_p^3}{L^3}$. The fluid force acting on the particle is aligned with the mean flow, so that $\mathbf{F}_p = F_{p,z} \mathbf{e}_z$. It is customary to define the normalized fluid-particle force as

$$\bar{F} = \frac{F_{p,z}}{F_{St}}, \quad (1.53)$$

where $F_{St} = 3\pi\mu d_p U_0$ is the drag force acting on an isolated sphere in Stokes regime. This problem was addressed theoretically by Zick and Homsy [160] who reported analytical values for $\bar{F}$ at different volume fractions and for different types of periodic networks. Numerically, the volume fraction is modified by changing the size L of the cubic domain and the maximal volume fraction is reached at $\phi_s = \frac{\pi}{6}$ when $L = d_p$. The Reynolds number is set to $\text{Re}_p = 0.01$ to be in the Stokes regime. In Figure 1.18, our results for the normalized fluid force acting on a sphere in a SC network are compared to the analytical values of Zick and Homsy [160], showing a good agreement over the whole range of solid fractions.

Since this problem has an analytical solution, it is also used to evaluate the convergence properties of our method in 3-D. Multiple simulations have been performed in dense ($\phi_s = \frac{\pi}{6} \simeq 0.524$) and dilute ($\phi_s = 0.125$) regimes at various grid resolutions. Figure 1.19a shows the convergence of the error made on $\bar{F}$ with respect to the analytical solution for the two solid fractions. It appears that the error decreases quadratically with the resolution, as previously observed by Breugem [15] for a retraction distance $r_d = 0.3h$ (while the same author reports a first-order accuracy when $r_d = 0$). It can also be inferred from Figure 1.19a that, for the same resolution, the error made on $\bar{F}$ is larger at higher ϕ_s (the sudden drop of the convergence curve for $\phi = 0.524$ is expected to be a statistical bias). This observation confirms that a finer resolution should be used for dense particle flows than for dilute flows. In Figure 1.19b, we plot the maximum value (L_∞ error) of the norm of the vector $\mathbf{U}_l$ among all Lagrangian points as a function of the resolution and normalized by $U_0/(1 - \phi_s)$. An exact enforcement of the boundary condition should result in $\mathbf{U}_l = 0$ since the particle has zero velocity. As for the force, the absolute error on $\mathbf{U}_l$ increases with ϕ_s , but the order of spatial convergence is here reduced to one. Indeed, the interpolation-spreading procedure needed by the IBM is known to be first-order accurate and it is expected that this

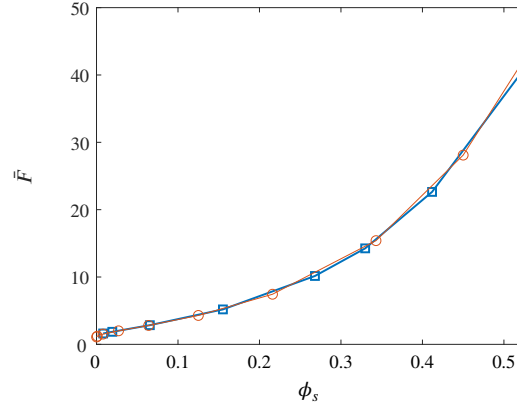


Figure 1.18: Normalized drag force acting on a sphere in a simple cubic array in Stokes regime: comparison between our results ($\square$) and the analytical solution of Zick and Homsy [160] ($\circ$).

feature will be evidenced by the more challenging convergence of a L_∞ -type error. To summarize, it seems that a well-chosen value for the retraction distance partly cancels the error induced by the interpolation-spreading operations and leads to an apparent second-order accuracy of the IBM for "averaged" quantities such as the force, but the intrinsic first-order accuracy of the IBM can be observed on more rigorous diagnostics.

This test case is also used to evaluate the influence of the multidirect forcing algorithm described in Section 1.2.2 on the accuracy of the solution. Figure 1.20a shows that the maximum of the error made on $\|U_f\|$ decreases rapidly as the number of MDF iterations increases, although between $M = 5$ and $M = 10$ the benefit provided by additional iterations is limited. On the other hand, Figure 1.20b shows that the time spent in the IBM routine increases almost linearly with the number of iterations. Therefore, using $M = 3$ appears as a good compromise between the gain in accuracy and the computational overhead induced by the interpolation-spreading operations.

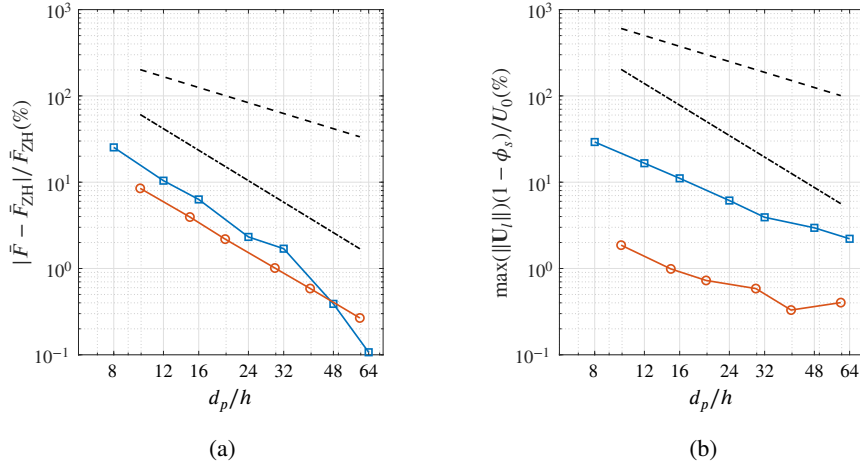


Figure 1.19: Stokes flow past a simple cubic array of spheres: convergence of (a) the error on the normalized drag force and (b) the maximum error in the norm of the Lagrangian velocity $\|\mathbf{U}_l\|$ at solid fractions $\phi_s = \pi/6 \approx 0.524$ ($\blacksquare$) and $\phi_s = 0.125$ ($\circ$). The first (--) and second (-.-) order convergence lines are also shown for comparison.

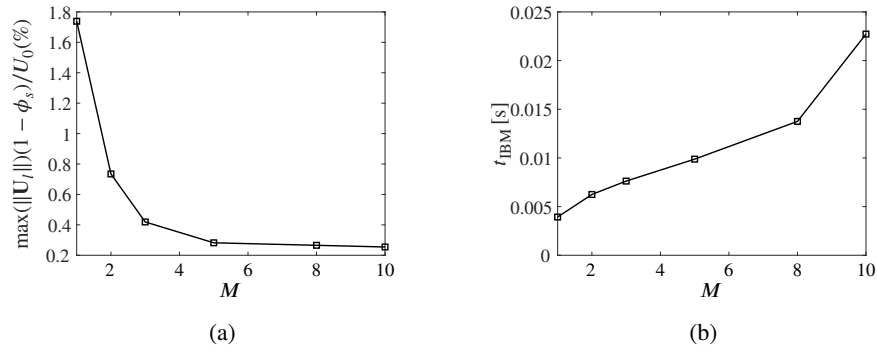


Figure 1.20: Impact of the number of multidirect forcing iterations on (a) the maximum error made on $\|\mathbf{U}_l\|$ and (b) the mean time spent in the IBM solver per time step.

1.5.3 Sedimentation of a sphere in a cavity

To validate the fluid-structure interaction part of the method, we first reproduce numerically the experiment of ten Cate et al. [130] who studied the settling of a single sphere in a box filled with silicon oil. The particle has a diameter $d_p = 15$ [mm] and a density $\rho_s = 1120$ [kg/m³]. The box has dimensions 100 [mm] x 100 [mm] x 160 [mm] and the spherical particle is released from rest with its lowest point located at 120 [mm] from the bottom of the domain. Different types of silicon oils were used to achieve terminal Reynolds numbers ranging from 1.5 to 31.9. The simulation parameters are detailed in Table 1.2⁵. The resolution $N_d = 18$ is kept constant for all simulations. In Figure 1.21a, it can be seen that our method is able to accurately reproduce the trajectory of the falling particle at the different terminal Reynolds numbers. The evolution of the vertical velocity w_p of the particle is also reported in Figure 1.21b, in good agreement with the experimental data.

ρ_{f0} [kg/m ³]	μ [10 ⁻³ Pa s]	U_t [m/s]	Re_t
970	373	0.038	1.5
965	212	0.060	4.1
962	113	0.091	11.6
960	58	0.128	31.9

Table 1.2: Physical parameters for the sedimentation of a sphere in a box filled with silicon oil (taken from [130]).

⁵The terminal velocity reported in the table correspond to the values given by ten Cate et al. [130]

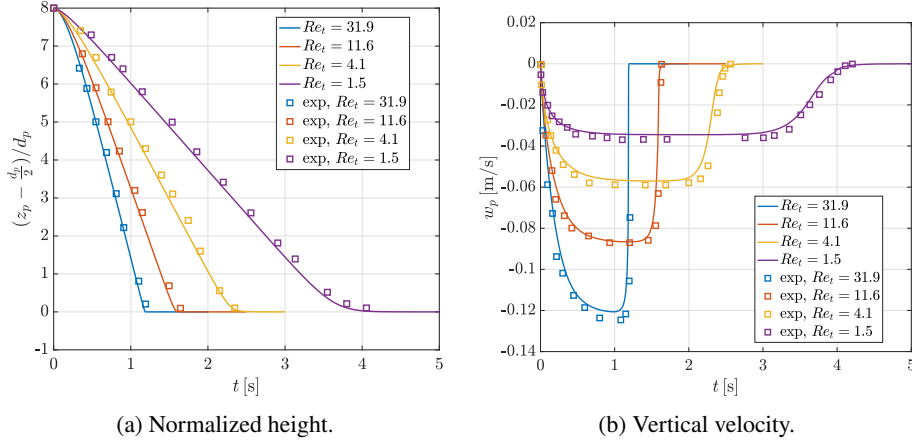


Figure 1.21: Sedimentation of a sphere in a box filled with silicon oil: time evolution of (a) the height and (b) the vertical velocity of the sphere for different terminal Reynolds numbers. Comparison between the results obtained with our IBM (solid line) and the experimental results from ten Cate et al. [130] (squares).

1.5.4 Normal approach between two spheres

Our collision model described in Appendix A combines a soft-sphere model to separate two particles (or a particle and a wall) once they overlap, and a lubrication model to recover correct hydrodynamic forces when the gap between the two particles (or between the particle and the wall) becomes too small (smaller than the grid size). As detailed in Section A.3, the lubrication model relies on three parameters: ϵ_0 , ϵ_1 and ϵ_2 . The first parameter ϵ_0 is the most critical one as it triggers when the lubrication correction is turned on. It must also be noted that ϵ_0 should be a function of the resolution since, when the grid is refined, the IBM should be able to correctly capture the forces for smaller gap widths. In [11], the authors suggest that $\frac{h}{R}$ is a good estimate for ϵ_0 . For a resolution $\frac{R}{h} = 8$, it yields $\epsilon_0 = 0.125$. In [18] and [14], the authors use a significantly smaller value, $\epsilon_0 = 0.025$, for the same resolution. To calibrate ϵ_0 , and similarly to what is done in those studies, we consider the normal approach of two spheres of equal radius and opposite velocities in Stokes regime for different separation distance δ . The two particles are located at $(0, 0, \pm\delta/2)$ and their velocity is set to $(0, 0, \mp U)$. The particle Reynolds number is $Re_p = \frac{d_p U}{\nu} = 0.1$. The magnitude of the velocity field is shown in Figure 1.22 for two spheres separated by a normalized gap $\epsilon = \frac{\delta}{R} = 0.2$. By decreasing the gap width between the two particles, we can estimate the value of the normalized gap ϵ_0 below which the IBM fails to capture

the correct forces. In Figure 1.23, we compare the force experienced by each particle to the analytical solution of Brenner [13]. Without lubrication correction, the fluid forces are underestimated below $\epsilon \simeq 0.05$. By applying the lubrication correction with $\epsilon_0 = 0.05$, we recover nicely the reference solution. We also tested $\epsilon_0 = 0.075$, but it appears that, in this case, the lubrication correction is turned on too early and the fluid forces are overestimated. Finally, regarding the two remaining parameters of the model, we stick to the values proposed in [14] that the authors derived from a thorough collision study, namely $\epsilon_1 = 0.001$ and $\epsilon_2 = 0.01$. The same parameter values are used for particle-wall collisions.

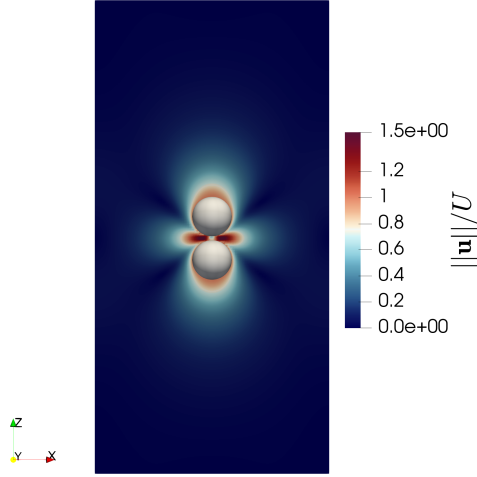


Figure 1.22: Normal approach of two spheres of equal size and opposite velocities $(0, 0, U)$ and $(0, 0, -U)$: velocity field magnitude.

1.5.5 Particle-wall collision

We now investigate the ability of our soft-sphere model to reproduce reference results for particle-wall collisions. A distinction is made in the literature between *dry* and *wet* collisions. Dry collisions refer to particle-particle and particle-wall contacts where the hydrodynamic interactions are negligible. Conversely, wet collisions correspond to contacts occurring in a viscous liquid where viscous dissipations and added mass

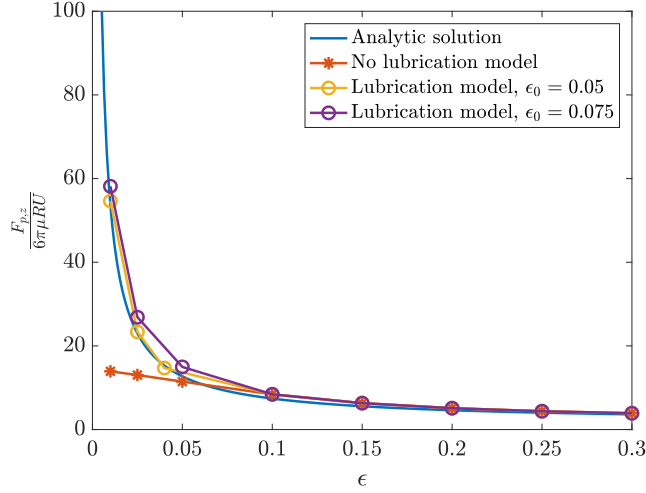


Figure 1.23: Hydrodynamic force experienced by two approaching spheres with and without lubrication correction. Present results are compared to the analytical solution of Brenner [13].

effects are significant. Both kinds of contacts are considered in the following validation procedure.

Dry oblique collision

In the case of a dry collision, energy is dissipated through mechanical contacts only and the energy dissipation can be quantified by the normal restitution coefficient e_n . In an oblique collision, the particle approaches the wall with an incidence angle ϕ_{in} and bounces with a rebound angle ϕ_{out} . Walton's theory [150] detailed in Appendix A.1 allows to calculate post-collision quantities and therefore the effective rebound angle. We reproduce here Joseph and Hunt's [64] experiment of glass spheres with density $\rho_s = 2450[\text{kg/m}^3]$ hitting a wall in ambient air. The normal and tangential restitution coefficients are $e_n = 0.97$ and $e_t = 0.39$ respectively, and the Coulomb's friction coefficient is $\mu_c = 0.1$. In Figure 1.24, we report values of $\Psi_{out} = \tan(\phi_{out})$ as a function of $\Psi_{in} = \tan(\phi_{in})$ using the standard soft-sphere model (as detailed in [144, 26]) and the more recent Costa's variant [18]. Our results are compared to Walton's theoretical model [150], to Costa et al. numerical results [18] and to Joseph and Hunt's experimental results [64]. It appears that the standard version of the soft-sphere model has trouble reproducing the transition zone between sticking (low angle of attack, $\Psi_{in} < \Psi_{in}^*$) and sliding (larger angle of attack, $\Psi_{in} > \Psi_{in}^*$) regimes. The normal

component of the rebound velocity is correctly captured by both models, but the tangential rebound velocity is overestimated while the rotational velocity induced by the contact is underestimated by the standard model. On the contrary, Costa's variant, which differs from the original model in the definition of the tangential unit vector and in the way the tangential displacement is saturated in the sliding regime, is able to capture correctly the sticking-sliding transition zone. Based on these observations, we chose to keep Costa's variant of the soft-sphere model for all the simulations presented in this work.

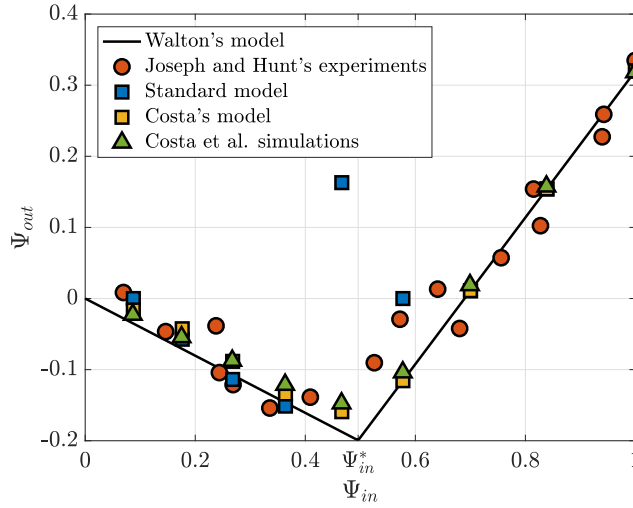


Figure 1.24: Dry oblique collision of a sphere onto a wall. Post-collisional quantity Ψ_{out} is obtained for different incident angles using the standard and Costa's soft-sphere model. Results are compared to Walton's theoretical model [150], Joseph and Hunt's experiments [64] and Costa's own numerical results [18].

Wet normal collision

To validate the coupling between our immersed boundary method and the soft-sphere collision model, we consider the experiment of Gondret et al. [52] of a sphere immersed in a viscous liquid and colliding onto a planar surface under the action of gravity, $\mathbf{g} = -9.81\mathbf{e}_z$. The fluid is a RV10 oil with density $\rho_f = 935 \text{ [kg/m}^3\text{]}$, and viscosity $\mu = 10 \times 10^{-3} \text{ [Pa s]}$. The sphere is made of steel with density $\rho_s = 7800 \text{ [kg/m}^3\text{]}$ and has a diameter $d_p = 3 \text{ [mm]}$. The normal restitution coefficient is $e_n = 0.97$. The computational domain is a closed container with dimensions $L_x \times L_y \times L_z =$

$12d_p \times 12d_p \times 30d_p$ and the sphere is released at $z_p = L_z - 1.5d_p$. The calibration of the collision model parameters is provided in Section A.2.3 of Appendix A. We compare in Figure 1.25 the trajectory of the bouncing sphere obtained from our simulations to the experimental results of Gondret et al. [52]. Simulations have been performed with different sets of parameters reported in Table 1.3. Namely, we investigated the sensitivity of the results by changing the fluid time step Δt , the sub-time stepping ratio n_{ss} and the number K_N of fluid time steps during a collision. By decreasing Δt or K_N , we decrease the total duration of the collision $T_n = K_N \Delta t$ and the collision is made stiffer since $k_n \sim \frac{1}{T_n^2}$ increases (see Eq. (A.44)). However, a stiffer collision also requires a smaller fluid time step to let the flow adapt to the abrupt changes in the particle velocity. Hence K_N must be large enough as to capture the collision correctly, and the corresponding fluid time step Δt must be small enough to allow the flow to adapt. It must be acknowledged that a significant gap is observed between our results and the results of Gondret et al. [52]. The fluid drag force seems overestimated by our simulations just after the rebound. Costa et al. [18] also report a strong sensitivity of their results on the time step and collision parameters. According to these authors, and following the earlier works of Kempe et al. [65], the discrepancy is caused by a loss of conservation properties of the IBM interpolation kernels when the stencils of some Lagrangian points overlap with another particle or with a wall. The cure proposed in [65] is to remove the problematic Lagrangian points from the forcing scheme when the distance between two particles or a particle and a wall is less than the grid size h . We tried to reproduce this strategy, but the results did not show any improvement. We can however discuss the sensitivity of our results to the numerical parameters. The simulation S1 in Table 1.3 is considered as the baseline. By decreasing K_N from 10 to 2 (S2), the overestimation of the drag is even more severe, since the stiffness of the collision has been increased while keeping the same time step. In S3, we have instead increased K_N by a factor 2, so that the collision is made softer and resolved over a longer time. The trajectory of the sphere appears to be slightly better predicted, although the drag overestimation is still significant. Then, we evaluated the influence of the solid sub-time stepping by increasing n_{ss} from 10 to 20 (S4). The trajectories obtained from simulations S1 and S4 are superimposed in Figure 1.25, which shows that the solid time step is already sufficiently small as to correctly capture the collision forces. In S5, the collision time T_n is the same as in S1 (and therefore the stiffness), but the time step Δt has been reduced by a factor 2. The trajectory of the sphere seems slightly better predicted, which is expected since the stiffness is unchanged but the time step is reduced. Clearly, there is room for improvement and we should further investigate

the sensitivity of our combined immersed boundary/soft-sphere model to the different numerical parameters in order to better match experimental data.

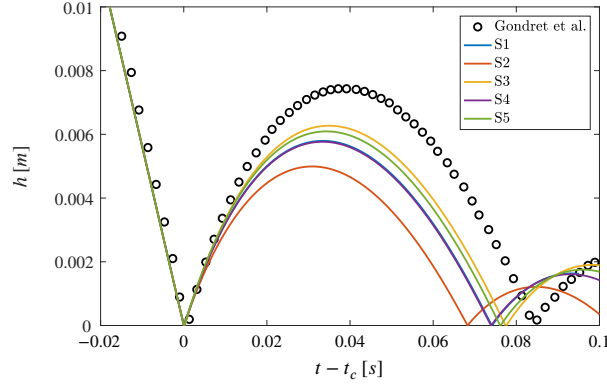


Figure 1.25: Trajectory of a steel sphere immersed in a RV10 oil bouncing on a plane. Sensitivity analysis to the numerical parameters reported in Table 1.3 and comparison with the experimental results of Gondret et al. [52].

	Δt [s]	n_{ss}	K_N	$T_n = K_n \Delta t$ [s]
S1	1×10^{-5}	10	10	1×10^{-4}
S2	1×10^{-5}	10	2	2×10^{-5}
S3	1×10^{-5}	10	20	2×10^{-4}
S4	1×10^{-5}	20	10	1×10^{-4}
S5	5×10^{-6}	20	20	1×10^{-4}

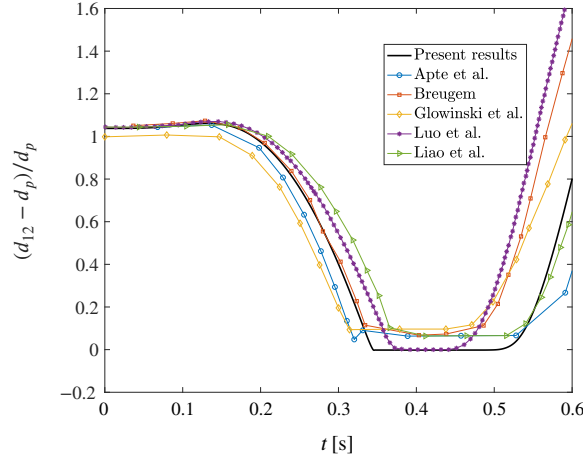
Table 1.3: Numerical parameters used in the sensitivity study to reproduce the experiment of Gondret et al. [52].

1.5.6 Drafting-kissing-tumbling of two spheres

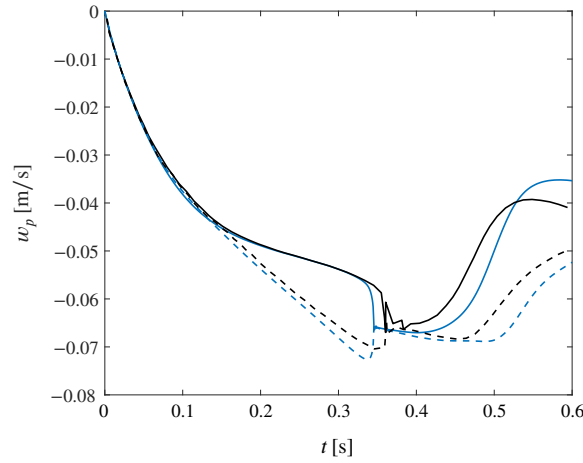
The DKT phenomenon examined in two dimensions in Section 1.4.2 is now reproduced in three dimensions. Two spheres of diameter $d_p = 1.677711 \times 10^{-3}$ [m] are placed above each other in a cavity with dimensions 0.1 [m] $\times$ 0.1 [m] $\times$ 0.4 [m]. The two particles are initially at rest and positioned at $(0.0505, 0.0505, 0.35)$ [m] and $(0.0495, 0.495, 0.316)$ [m]. The slight offset in the transversal position of the two particles is used to trigger the drafting-kissing-tumbling phenomenon. The density of

the solid and the fluid are $\rho_s = 1140[\text{kg/m}^3]$ and $\rho_f = 1000[\text{kg/m}^3]$, respectively. The fluid viscosity is $\mu = 1 \times 10^{-3}[\text{Pa s}]$ and the gravitational acceleration is $\mathbf{g} = -9.81\mathbf{e}_z[\text{m/s}^2]$.

Figure 1.26a shows the gap between the two falling spheres as a function of time, where $d_{12} = \|\mathbf{x}_1 - \mathbf{x}_2\|$ is the distance between the two particle centers. In the first part of the fall, the different results of the literature are close to each other, but they differ quite significantly regarding the duration of the contact, which is very sensitive to the collision model. Except for our results and those reported by Luo et al. [77] who also used a soft-sphere model, other studies use a simpler model based on a repulsion potential and originally proposed by Glowinski [51]. This model does not allow the particles to overlap, so that the gap between them never reaches exactly zero. In Figure 1.26b, the time evolution of the vertical velocity component w_p of the two spheres is compared to the data of Breugem [15]. As for the two-dimensional counterpart, the agreement is very satisfactory in the first part until the trailing particle catches the leading one and the curves are qualitatively similar in the second part.



(a) Gap between the spheres: comparison between our results and those reported by Apte et al. [6], Breugem [15], Glowinski et al. [51], Luo et al. [77] and Liao et al. [73].



(b) Vertical velocity component of the leading (solid line) and trailing (dashed line) particles. Present results (—) are compared to those reported by Breugem (—) [15].

Figure 1.26: Drafting-kissing-tumbling of two spheres in a box: time evolution of (a) the gap between the spheres and (b) the vertical velocity component of the spheres.

1.5.7 Heat transfer with forced convection past a sphere

Non-reactive case: sphere with constant temperature

The next step in the 3-D validation procedure is to consider non-isothermal flows. The heat transfer resulting from the flow past a sphere at a different temperature than the fluid has been studied both experimentally [80, 153] and numerically [41, 126, 136]. We reproduce here this benchmark by placing a sphere in a channel with dimensions $16d_p \times 8d_p \times 8d_p$, the sphere being located at a distance $3d_p$ from the inflow. The sphere has a fixed temperature T_p and the inflow is at a temperature T_∞ . On the side walls, we impose slip and adiabatic conditions on the velocity and temperature fields, respectively. The Prandtl number is unity. The efficiency of the heat transfer between the sphere and the surrounding fluid is quantified by the Nusselt number

$$\text{Nu} = \frac{Q_p}{k_f \pi d_p (T_p - T_\infty)} = \frac{h_f d_p}{k_f}, \quad (1.54)$$

where $h_f = \frac{Q_p}{\pi d_p^2 (T_p - T_\infty)}$ is the heat transfer coefficient (in $[W/(m^2 K)]$). In Stokes regime, the limit of the Nusselt number is 2. At finite Reynolds number, various correlations have been proposed in the literature to evaluate Nu as function of the Reynolds and Prandtl numbers:

$$\begin{aligned} \text{Ranz and Marshall [80]} \quad \text{Nu} &= 2.0 + 0.6 \text{Re}_p^{1/2} \text{Pr}^{1/3}, & (1.55) \\ &10 \leq \text{Re}_p \leq 1000, \text{Pr} \geq 0.7, \end{aligned}$$

$$\begin{aligned} \text{Whitaker [153]} \quad \text{Nu} &= 2.0 + \left(0.4 \text{Re}_p^{1/2} + 0.06 \text{Re}_p^{2/3} \right) \text{Pr}^{2/5}, & (1.56) \\ &3.5 \leq \text{Re}_p \leq 7.6 \times 10^4, 0.7 \leq \text{Pr} \leq 380, \end{aligned}$$

$$\begin{aligned} \text{Feng and Michaelides [41]} \quad \text{Nu} &= 0.992 + \text{Pe}^{1/3} + 0.1 \text{Re}_p^{1/3} \text{Pe}^{1/3}, & (1.57) \\ &0.1 \leq \text{Re}_p \leq 4000, 0.2 \leq \text{Pr} \leq 2000, \end{aligned}$$

where $\text{Pe} = \text{Pr} \text{Re}_p$ is the Péclet number. The first two correlations were obtained experimentally while the third one was derived numerically. We report in Figure 1.27 our results for the steady-state value of the Nusselt number for a range of Reynolds numbers and for two resolutions $N_d = (16, 32)$. Our results are in good agreement with Feng and Michaelides correlation, which happens to be based on first principles unlike the other two correlations. The comparison is even better when the resolution is increased.

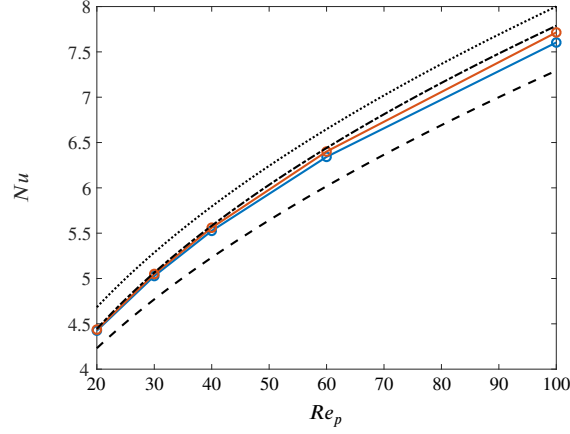


Figure 1.27: Heat transfer with a sphere in forced convection: evolution of the Nusselt number as a function the Reynolds number obtained from our PR-DNS data at resolutions $N_d = 16$ ($\circ$) and 32 ($\circ$). Comparison with the correlations proposed by Ranz and Marshall [80] ($\cdots$), Whitaker [153] ($-$) and Feng and Michaelides [41] ($- \cdot -$).

Mass transfer limited exothermic reaction

We now consider the case of a very fast exothermic chemical reaction $A \longrightarrow B$ at the surface of a stationary sphere. This problem was investigated numerically by Deen et al. [24]. The temperature of the particle is free to evolve as a result of the balance between the interfacial heat flux and the reaction heat source term (Eq. (1.10)). Since the reaction is very fast, the effective reaction rate will be limited by mass transfer, so that the heat source term reads

$$Q_s = J_{A,p}(-\Delta H), \quad (1.58)$$

where ΔH is the reaction heat and $J_{A,p}$ is the interfacial mass flux of reactant A . At steady-state, $\frac{dT_p}{dt} = 0$ and Eq. (1.10) simplifies as

$$0 = Q_p + J_{A,p}(-\Delta H), \quad (1.59)$$

which means that all the heat released by the reaction is evacuated by the fluid. The heat and mass fluxes can be expressed in terms of the heat and mass transfer coefficients and the corresponding driving forces,

$$0 = h_f (T_\infty - T_p) + h_m (C_{A,\infty} - C_{A,p}) (-\Delta H), \quad (1.60)$$

where h_m is the mass transfer coefficient and $C_{A,\infty}$ is the concentration of species A in the inflow. Because the reaction rate is limited by mass transfer, the surface of the particle is free of any reactant, i.e. $C_{A,p} = 0$, and the steady-state temperature at the surface of the particle can be expressed as

$$T_p = T_\infty + \frac{h_m}{h_f} C_{A,\infty} (-\Delta H) = T_\infty + \frac{\text{Sh}}{\text{Nu}} \text{Le}^{-1} \frac{C_{A,\infty} (-\Delta H)}{\rho_{f0} c_{p,f}}, \quad (1.61)$$

where $\text{Sh} = \frac{h_m d_p}{D_f}$ ⁶ is the Sherwood number characterizing the efficiency of the mass transfer and $\text{Le} = \frac{\text{Sc}}{\text{Pr}} = \frac{\alpha_f}{D_f}$ is the Lewis number. Thanks to the analogy between heat and mass transfer, the correlations (1.55), (1.56) and (1.57) can also be used to obtain the Sherwood number as a function of the Reynolds and Schmidt numbers (in replacement of the Prandtl number).

The simulation parameters are taken from [24] and reported in Table 1.4. The sphere is positioned at a distance $2d_p$ from the inflow and it is centered in the transverse directions. The Reynolds number varies between 30 and 240 by changing the inflow velocity, the Prandtl number is $\text{Pr} = 0.8$ and the Schmidt number is $\text{Sc} = 1$. The resolution of the grid increases with the Reynolds number from $N_d = 24$ at $\text{Re}_p = 30$ to $N_d = 48$ at $\text{Re}_p = 240$. In Table 1.5, we compare our results for the steady-state temperature rise $\Delta T = T_p - T_\infty$ with the results of Deen et al. [24] and with the values obtained by the combination of Eqs. (1.61) and (1.57). The agreement is very good, showing the ability of the present method to reproduce a more complex test case involving coupled heat and mass transfer at moderate Reynolds numbers.

⁶Species A and B are assumed to have the same fluid-phase diffusivity D_f so that we omit the species index.

Particle diameter	d_p	0.015 [m]
Resolution	$N_d = \frac{d_p}{h}$	(24, 24, 32, 48)
Domain size	$L_x = L_y = L_z$	$8d_p = 0.12$ [m]
Fluid density	ρ_{f0}	1 [kg/m ³]
Fluid viscosity	μ	2×10^{-5} [Pa s]
Fluid species diffusivity	D_f	2×10^{-5} [m ² /s]
Fluid heat capacity	$c_{p,f}$	1000 [J/(kg K)]
Fluid thermal conductivity	k_f	0.025 [W/(m K)]
Solid density	ρ_s	1 [kg/m ³]
Solid heat capacity	$c_{p,s}$	1000 [J/(kg K)]
Reaction heat	ΔH	−100 000 [J/kg]
Inlet velocity	U_∞	(0.04, 0.08, 0.16, 0.32) [m/s]
Inlet temperature	T_∞	293 [K]
Inlet concentration for species A	$C_{A,\infty}$	1 [kg/m ³]

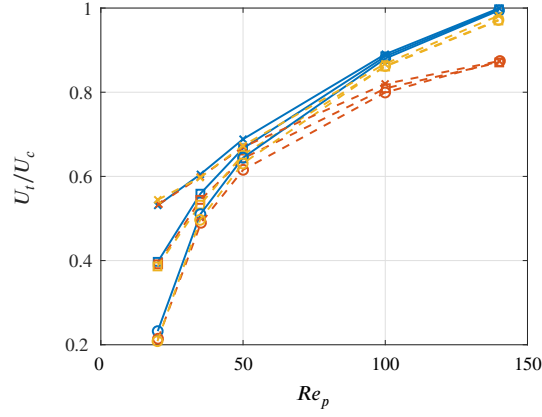
Table 1.4: Physical and numerical parameters for the flow past a fixed sphere with very fast exothermic surface reaction.

Re_p	ΔT [K]		
	Feng and Michaelides [41] (Eq. (1.57))	Deen et al. [24]	Present results
30	84.9	85.0	84.9
60	85.2	85.4	85.3
120	85.4	85.8	85.8
240	85.6	86.1	86.1

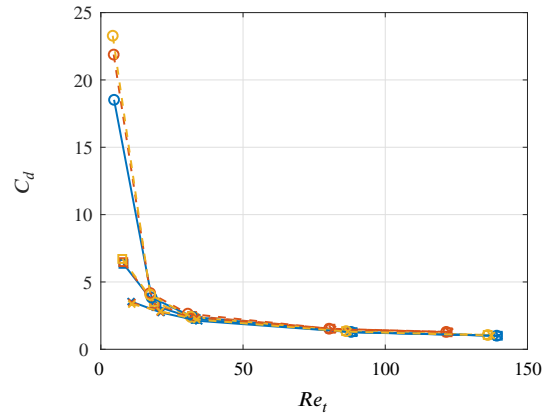
Table 1.5: Temperature rise resulting from a mass transfer limited exothermic surface reaction at the surface of a sphere in forced convection. Our DNS results are compared to those reported by Deen et al. [24] and to the theoretical value obtained using Feng and Michaelides correlation [41] for the Nusselt and Sherwood numbers.

1.5.8 Sedimentation of a buoyant sphere in a semi-infinite channel

To validate the coupling between momentum and heat transfer with fluid-structure interaction, we consider the test case proposed by Dan et al. [21] of a buoyant sphere settling in a semi-infinite channel. The channel has dimensions $4d_p \times 4d_p \times 20d_p$ and the sphere is released from rest at $10d_p$ from the bottom of the channel. To prevent the particle to reach the bottom of the domain, the computational box and the whole solution fields are translated upwards when the particle is at distance $6d_p$ from the bottom of the box. The reference velocity of the problem is defined by Eq. (1.42). The density ratio ρ_r between the solid and the fluid phases varies in the range $[1.00204, 1.1]$. Since all other physical parameters are kept constant, changing the density ratio make Re_p vary between 20 and 140. Simulations are performed for three Grashof numbers: 0, 100 (hot particle) and -100 (cold particle) and the Prandtl number is 1. A resolution $N_d = 24$ is used for all simulations. Figure 1.28a shows the evolution of the terminal velocity of the sphere with the characteristic Reynolds number and Figure 1.28b reports the drag coefficient C_d defined by Eq. (1.43) as a function of the terminal Reynolds number. We observe qualitatively the same thermo-mechanical phenomenon as the one detailed in 2-D: a sphere at a higher temperature than the fluid will reach a lower terminal velocity as the natural convection effects tend to counteract gravity while a sphere colder than the fluid will fall faster as natural convection acts in the same direction as gravity. Yet, a noticeable difference can be observed between Figures 1.12a and 1.28a for the case at $Gr = -100$: for the sphere, U_t is monotonically increasing with Re_p (i.e. with the density ratio) whereas for the cylinder, U_t was decreasing for Re_p in the range $[12.4, 27.8]$ and then increasing again. As noted by Dan et al. [21], this difference might be attributed to stronger confinement effects in 3-D given the size of the transverse dimension ($16d_p$ in 2-D vs. $4d_p$ in 3-D) or to intrinsic three-dimensional effects. In any case, our results compare very well with those reported by Majlesara et al. [78] who used an IBM similar to ours while Dan et al. [21] obtain smaller values for the terminal velocity at high Reynolds number.



(a)



(b)

Figure 1.28: Sedimentation of a sphere in a semi-infinite channel at $Gr = 0$ ($\blacksquare$), $Gr = 100$ ($\bullet$) and $Gr = -100$ ($\times$): (a) terminal velocity as a function of Re_p and (b) drag coefficient as a function of Re_t . Our results are compared to those reported by Dan et al. [21] (respectively $\square$, $\circ$ and $\times$) and Majlesara et al. [78] (respectively $\square$, $\circ$ and $\times$).

1.6 3-D parallelization

In order to perform three-dimensional resolved simulations containing more than $\mathcal{O}(10^3)$ particles, it is crucial to obtain an efficient parallelization of the whole numerical method. We discuss in this section the parallelization strategy that was set-up for the IBM and DEM solvers and we evaluate its performance through detailed scaling studies.

1.6.1 Combined master-slaves / cell linked list strategy

Regarding the background Navier-Stokes solver, the parallelization is performed using a classical domain decomposition and the Poisson equation is solved with an improved multigrid algorithm [31]. To discuss the parallelization strategy of the features added to the 3-D solver, we summarize in Algorithm 1 the global IBM-DEM numerical scheme, omitting scalars for simplicity.

The solid phase parallelization procedure combines a master-slaves strategy (M-S) similar to the one developed by Uhlmann in [140] and a Cell Linked List (CLL) algorithm [81] to search for particle-particle collisions. In the present case, the cells result from the decomposition of the physical domain used for the parallelization of the Navier-Stokes solver. Figure 1.29 illustrates in two dimensions the combined M-S/CLL algorithm. The reference process is identified by the indices (I, J) in the partitioning of the domain and it possesses 8 neighbor processes (26 in three dimensions). The process (I, J) is the master of the red particles while it is a slave for the blue particles. The position and velocity of a particle are updated by its "master", i.e. the process whose domain contains the centroid of the particle. Due to their finite size, particles will frequently span over two or more processes. These processes, the "slaves", will perform part of the calculations needed to solve the dynamics of the particle and transfer their result back to the master. In particular, each slave will handle the IBM interpolation-spreading operations for the Lagrangian points located in its domain and communicate to the master its local portion of the Lagrangian velocity vector $\mathbf{U}_l^{**}$. The master process of each particle can then evaluate hydrodynamic and contact forces and solve the particle dynamics. In the CLL algorithm, the process (I, J) is aware of the positions and velocities of all coloured particles in Figure 1.29 (including the green ones), i.e. the particles whose center is included in its domain or the domain of one of its neighbors, without necessarily overlapping. These particles are stored in the list of the reference process. At each solid sub-time step, each process searches for existing collisions between the particles located in its domain and the other particles contained in the list. This implies that a particle cannot span beyond the direct neighbors of its

Algorithm 1: Global IBM-DEM numerical scheme

$$\mathbf{U}_p^n(\mathbf{X}_I) = \mathbf{u}_p^n + \mathbf{\Omega}_p^n \wedge \mathbf{r}_I \quad (1.62a)$$

$$\mathbf{u}^* = \mathbf{u}^n + \Delta t \left(\left(\frac{3}{2} \mathbf{C}_u^n - \frac{1}{2} \mathbf{C}_u^{n-1} \right) + \nu \nabla^2 \mathbf{u}^n - \frac{1}{\rho_{f0}} \nabla p^n + \mathbf{B}^n \right) \quad (1.62b)$$

Set: $\mathbf{u}^{*,0} = \mathbf{u}^*$ and $\mathbf{F}_I^{n,0} = 0$

for $k = 1 \rightarrow M$ do

$$\mathbf{U}_I^{*,k}(\mathbf{X}_I) = \sum_{\mathbf{x}} \mathbf{u}^{*,k-1}(\mathbf{x}) \delta_h(\mathbf{x} - \mathbf{X}_I) h^3 \quad (1.62c)$$

$$\mathbf{F}_I^{n,k}(\mathbf{X}_I) = \mathbf{F}_I^{n,k-1} + \frac{\mathbf{U}_p^n(\mathbf{X}_I) - \mathbf{U}_I^{*,k}(\mathbf{X}_I)}{\Delta t} \quad (1.62d)$$

$$\mathbf{f}^{n,k}(\mathbf{x}) = \sum_I \mathbf{F}_I^{n,k}(\mathbf{X}_I) \delta_h(\mathbf{x} - \mathbf{X}_I) \Delta V_I \quad (1.62e)$$

$$\mathbf{u}^{*,k} = \mathbf{u}^* + \Delta t \mathbf{f}^{n,k} \quad (1.62f)$$

end

$$\nabla^2 \Phi = \rho_{f0} \frac{\nabla \cdot \mathbf{u}^{**}}{\Delta t} \quad (1.62g)$$

$$\mathbf{u}^{n+1} = \mathbf{u}^{**} - \frac{\Delta t}{\rho_{f0}} \nabla \Phi \quad (1.62h)$$

$$p^{n+1} = p^n + \Phi \quad (1.62i)$$

$$\mathbf{F}_p^n = \rho_{f0} \left[- \sum_I \mathbf{F}_I^n \Delta V_I + \frac{1}{\Delta t} \left(\left\{ \int_{V_p} \mathbf{u} \, dV \right\}^{n+1} - \left\{ \int_{V_p} \mathbf{u} \, dV \right\}^n \right) - \int_{V_p} \mathbf{B}^n \, dV \right] \quad (1.62j)$$

$$\mathbf{M}_p^n = \rho_{f0} \left[- \sum_I (\mathbf{r}_I^n \wedge \mathbf{F}_I^n) \Delta V_I + \frac{1}{\Delta t} \left(\left\{ \int_{V_p} \mathbf{r} \wedge \mathbf{u} \, dV \right\}^{n+1} - \left\{ \int_{V_p} \mathbf{r} \wedge \mathbf{u} \, dV \right\}^n \right) - \int_{V_p} (\mathbf{r}^n \wedge \mathbf{B}^n) \, dV \right] \quad (1.62k)$$

Set: $\mathbf{u}_p^{k=0} = \mathbf{u}_p^n$, $\mathbf{\Omega}_p^{k=0} = \mathbf{\Omega}_p^n$, $\mathbf{x}_p^{k=0} = \mathbf{x}_p^n$, $\mathbf{q}_p^{k=0} = \mathbf{q}_p^n$

for $k = 1 \rightarrow n_{ss}$ do

Set: $\mathbf{u}_p^{k,l=0} = \mathbf{u}_p^{k-1}$, $\mathbf{\Omega}_p^{k,l=0} = \mathbf{\Omega}_p^{k-1}$, $\mathbf{x}_p^{k,l=0} = \mathbf{x}_p^{k-1}$, $\mathbf{q}_p^{k,l=0} = \mathbf{q}_p^{k-1}$, $l = 1$

do

$$\mathbf{F}_c^{k,l} = \mathbf{F}_c(\mathbf{x}_p^{k,l-1}, \mathbf{q}_p^{k,l-1}, \mathbf{u}_p^{k,l-1}, \mathbf{\Omega}_p^{k,l-1}) \quad (1.62l)$$

$$\mathbf{M}_c^{k,l} = \mathbf{M}_c(\mathbf{x}_p^{k,l-1}, \mathbf{q}_p^{k,l-1}, \mathbf{u}_p^{k,l-1}, \mathbf{\Omega}_p^{k,l-1}) \quad (1.62m)$$

$$\mathbf{u}_p^{k,l} = \mathbf{u}_p^{k-1} + \frac{\Delta t_s}{V_p \rho_s} \mathbf{F}_p^n + \frac{\Delta t_s}{V_p \rho_s} \frac{(\mathbf{F}_c^{k,l} + \mathbf{F}_c^{k-1})}{2} + \Delta t_s \frac{(\rho_s - \rho_{f0})}{\rho_s} \mathbf{g} \quad (1.62n)$$

$$\mathbf{\Omega}_p^{k,l} = \mathbf{\Omega}_p^{k-1} + \frac{\Delta t_s}{I_p} \mathbf{M}_p^n + \frac{\Delta t_s}{I_p} \frac{(\mathbf{M}_c^{k,l} + \mathbf{M}_c^{k-1})}{2} \quad (1.62o)$$

$$\mathbf{x}_p^{k,l} = \mathbf{x}_p^{k-1} + \frac{\Delta t_s}{2} (\mathbf{u}_p^{k,l} + \mathbf{u}_p^{k-1}) \quad (1.62p)$$

$$\mathbf{q}_p^{k,l} = \mathbf{q}_p^{k-1} + \frac{\Delta t_s}{2} \left(\frac{1}{2} \mathbf{Q}^{k,l} \bar{\mathbf{\Omega}}_p^{k,l} + \frac{1}{2} \mathbf{Q}^{k-1} \bar{\mathbf{\Omega}}_p^{k-1} \right) \quad (1.62q)$$

$l = l + 1$

while $\Delta \mathbf{x}_p = \|\mathbf{x}_p^{k,l} - \mathbf{x}_p^{k,l-1}\| < \epsilon$;

end

Set: $\mathbf{u}_p^{n+1} = \mathbf{u}_p^{k=n_{ss}}$, $\mathbf{\Omega}_p^{n+1} = \mathbf{\Omega}_p^{k=n_{ss}}$, $\mathbf{x}_p^{n+1} = \mathbf{x}_p^{k=n_{ss}}$, $\mathbf{q}_p^{n+1} = \mathbf{q}_p^{k=n_{ss}}$.

master process, i.e $d_p \leq 2L_{proc}$, where L_{proc} is the smallest dimension of the process domain. Also, the collision search algorithm requires each process to communicate to all its neighbors the new positions and velocities of the particles that it holds at each sub-time step of the solid solver. The number n_{ss} of solid sub-steps must therefore be kept reasonable to avoid excessive communications. A summary of the parallelization strategy is presented in Table 1.6, where one can identify who holds what quantity at different stages of the algorithm and the necessary communications.

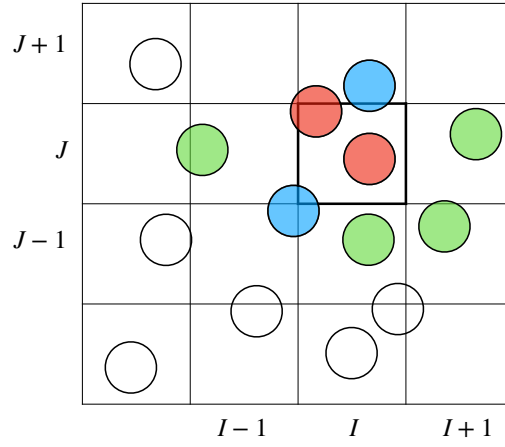


Figure 1.29: Schematic of the combined master-slaves / cell linked list algorithm parallelization strategy. The process (I, J) is a master for the red particles, a slave for the blue particles and a neighbor process for the green particles.

Operation	Result	Input	Who holds ?	Communication
(1.62a)	$\mathbf{U}_p^n(\mathbf{X}_l)$	$\mathbf{x}_p^n, \mathbf{u}_p^n, \mathbf{\Omega}_p^n, \mathbf{q}_p^n$	M+S (redundant)	-
(1.62c)	$\mathbf{U}_l^{*,*,k}$	$\mathbf{u}^{*,*,k}$	M+S (partial)	$\mathbf{U}_l^{*,*,k} : \text{M+S} \rightarrow \text{M+S (AllReduce)}$
(1.62d)	$\mathbf{F}_l^{n,k}$	$\mathbf{U}_l^{*,*,k}, \mathbf{U}_p^n(\mathbf{X}_l)$	M+S (redundant)	-
(1.62e)	$\mathbf{f}^{n,k}$	$\mathbf{F}_l^{n,k}$	M+S (partial)	-
pre-(1.62j)	-	-	-	$\int_{V_p} \mathbf{u}^n dV, \int_{V_p} \mathbf{B}^n dV : \text{S} \rightarrow \text{M}$
(1.62j), (1.62k)	$\mathbf{F}_p^n, \mathbf{M}_p^n$	$\mathbf{F}_l^n, \int_{V_p} \mathbf{u}^n dV, \int_{V_p} \mathbf{B}^n dV$	M	-
(1.62l), (1.62m)	$\mathbf{F}_c^k, \mathbf{M}_c^k$	$\mathbf{u}_p^{k-1}, \mathbf{\Omega}_p^{k-1}, \mathbf{x}_p^{k-1}, \mathbf{q}_p^{k-1}$	M	-
(1.62n)-(1.62q)	$\mathbf{u}_p^k, \mathbf{\Omega}_p^k, \mathbf{x}_p^k, \mathbf{q}_p^k$	$\mathbf{u}_p^{k-1}, \mathbf{\Omega}_p^{k-1}, \mathbf{x}_p^{k-1}, \mathbf{q}_p^{k-1}, \mathbf{F}_p^n, \mathbf{M}_p^n, \mathbf{F}_c^k, \mathbf{M}_c^k$	M	$\mathbf{u}_p^{k+1}, \mathbf{\Omega}_p^{k+1}, \mathbf{x}_p^{k+1}, \mathbf{q}_p^{k+1} : \text{M} \rightarrow \text{NGBRS}$
-	-	-	-	If master changes: transfer all body's data from M (old master) $\rightarrow$ M' (new master)

Table 1.6: Master-slaves parallelization strategy. M stands for the master process, S for the slave processes and NGBRS for the neighbor processes of the particle's master (i.e. larger set than only the slaves).

1.6.2 Performance

To assess the speedup achieved by the parallelization of the solid solver, we consider the case of a suspension of $N_p = 1000$ particles falling under the action of gravity in a 3-D periodic box of dimension L and in the presence of an external pressure gradient along the vertical direction to cancel the net fluid flow rate. This problem is described in more details in Section 4.4. The number of particles was chosen sufficiently large in order to see the impact of the parallelization of the solid solver. The resolution is set to $N_d = 16$. Due to memory constraints, the smallest number of processes required for the simulation had to be set to 32. Hence the speedup is here defined as the ratio between the time taken by the simulation on 32 processes and the time taken on n_{proc} processes:

$$\text{speedup} = \frac{t_{32}}{t_{n_{proc}}}. \quad (1.63)$$

We first present in Figure 1.30 the timings of the different parts of the whole solver when the number of processes is increased, both in absolute value (Figure 1.30a) and as a fraction of the CPU time per time step (Figure 1.30b). As expected, the Poisson solver is the most computationally expensive step (53.1 % of the CPU time using $n_{proc} = 32$). Yet, the parts devoted to the IBM and to the solid solver are also seen to be expensive, and roughly equally. At $n_{proc} = 32$, they cost respectively 20.6 % and 22.3 % of the total CPU time, i.e. their cumulative cost is slightly lower than that of the Poisson solver. It also appears that the ratio of the CPU time taken by the different parts of the solver remains fairly constant, although the contribution of the Poisson solver seems to slightly increase with the number of processes.

Figure 1.31 shows the speedup of the global solver and the individual speedups of the fluid and solid solvers as a function of the number of processes. The speedup of the solid solver happens to be slightly supra-linear between 32 and 256 processes and then flattens out. To understand this behavior, we plot in Figure 1.32 the speedup achieved by the different contributions of the solid solver, namely: the evaluation of the hydrodynamic forces, the DEM solver (including collision search), the master-slaves parallelization strategy (master-to-slaves and old to new master communications as well as communicators creation and destruction), the calculation of the solid mask (indicator function) and the update of the Lagrangian points. It can be observed that the calculation of the mask and the DEM part of the solid solver both show a supra-linear speedup. The complexity of the calculation of the mask fields (one by particle) is proportional to the number of particles owned by each processor multiplied by the

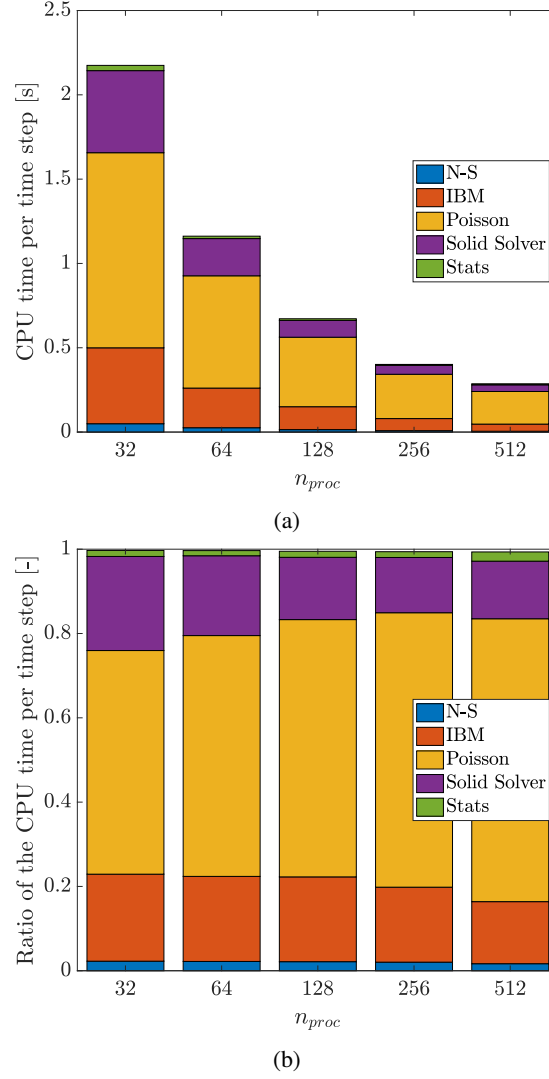


Figure 1.30: Mean time spent by the different contributions of the global solver for increasing values of n_{proc} (a) in absolute value and (b) relatively to the CPU time per time step.

size of the field:

$$t_{mask} \sim \frac{N_p}{n_{proc}} \times \frac{L^3}{n_{proc}} \sim \frac{1}{n_{proc}^2}, \quad (1.64)$$

which means that the time taken by the calculation of the mask fields decreases faster than $\frac{1}{n_{proc}}$. For the DEM solver, the search of collisions between the particles in the domain of the current process and those belonging to its neighbors is proportional to $\left(\frac{N_p}{n_{proc}}\right)^2$, which also explains the supra-linear speedup.

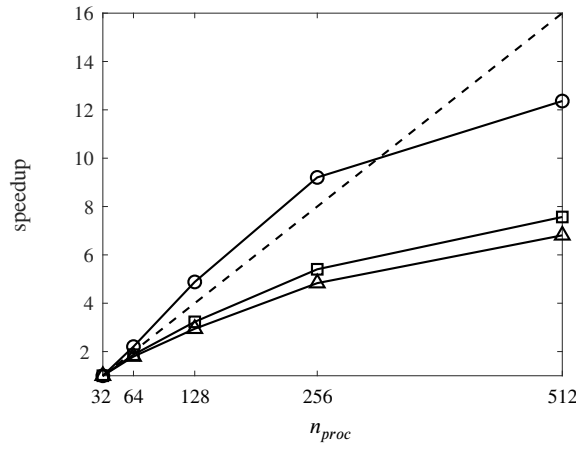


Figure 1.31: Speedup of the global solver (—○—), fluid solver (—□—) and solid solver (—△—) compared to the linear speedup (---).

Finally, Figure 1.33 shows the evolution of the mean CPU time spent in the different contributions of the solid solver. As already inferred from Figure 1.32, the time taken by these different steps decreases with n_{proc} , except for the master-slaves step which seems to take approximately the same amount of time. Inside the master-slaves contribution, the creation of new body-attached communicators appears to be the most time consuming operation. The time taken for the creation of these sub-communicators should scale as $\frac{N_p}{n_{proc}}$, but the larger amount of communications seems to mitigate this effect. Consequently, the time taken by the solid solver is mainly driven by the master-slaves operations at $n_{proc} = 512$ while the calculation of the mask fields and the DEM part are the dominant contributions at $n_{proc} = 32$.

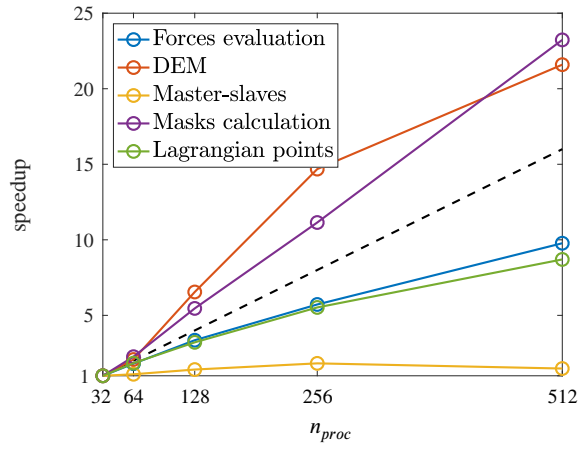
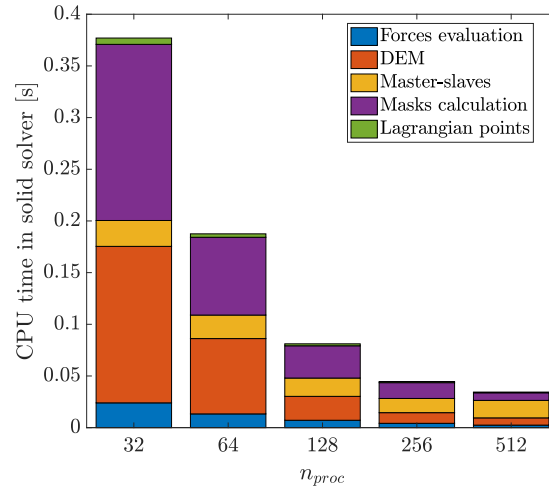
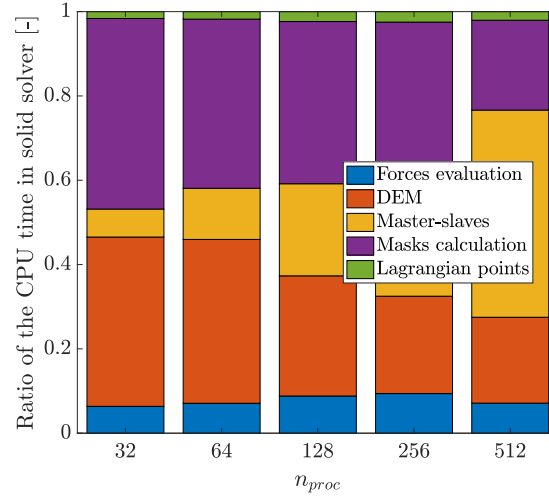


Figure 1.32: Speedup of the different steps in the solid solver compared to the linear speedup (---).



(a)



(b)

Figure 1.33: Mean time spent by the different contributions of the solid solver for increasing values of n_{proc} (a) in absolute value and (b) relatively to the CPU time spent in the solid solver.

1.7 Conclusions

This chapter was dedicated to the description and validation of the numerical method used to perform resolved simulations of particle flows in two and three dimensions. Our methodology is inspired from the improved direct-forcing immersed boundary method proposed by Breugem [15]. The IBM allows an efficient fluid-solid coupling by the addition of a continuous forcing term in the conservation equations of the fluid phase. A key ingredient of this method, and probably also one of its weak points, is the retraction distance r_d of the Lagrangian points from the surface of the particles. By setting $r_d = 0.3h$, we obtained close to second-order accuracy for averaged quantity such as forces, but the intrinsic first-order behavior of the IBM was recovered for L_∞ -type errors. The methodology is easily coupled to a DEM solver to update the positions and velocities of the moving particles. A combined soft-sphere/lubrication model is used to treat particle-particle and particle-wall collisions. We performed dedicated studies to validate the collision model and to evaluate the influence of different numerical parameters. The IBM was also used to enforce Dirichlet boundary conditions on scalar fields, namely temperature and species concentration fields. Then, different benchmarks were used to assess the accuracy of our method when gravity and natural convection effects play a role, both in 2-D and 3-D. Finally, we detailed the parallelization strategy of the 3-D solid solver, based on a master-slaves/cell linked list algorithm. Scaling studies showed the good performance of the global solver, opening the way for resolved simulations of a larger number of particles.

A microstructure-based model to predict fluid-particle forces in fixed particle arrays

In Fall 2020, the author had the opportunity to stay for two months at the Institut de Mécanique des Fluides de Toulouse (IMFT), France, under the kind supervision of Prof. Olivier Simonin. This chapter summarizes the outcome of this collaboration and is largely based on the article "Simulation of the flow past random arrays of spherical particles: Microstructure-based tensor quantities as a tool to predict fluid-particle forces" by B. Hardy, O. Simonin, J. De Wilde and G. Winckelmans published in International Journal of Multiphase Flow (2022) [55].

2.1 Introduction

As detailed in the Introduction of this thesis, particle-resolved simulation allows a "model-free" description of the fluid-particle coupling, but this approach is limited to small-scale systems. At larger scales, the (unresolved) Euler-Lagrange (EL) approach, also called CFD-DEM hereafter, or the Euler-Euler (EE) approach must be considered. In both cases, the interfacial stresses are no longer captured by the simulation. It is therefore of crucial importance to provide accurate and reliable relations for the fluid-particle force over a wide range of macro-scale parameters.

The first drag force constitutive relations were derived empirically [33, 152], but the recent advances of PR-DNS have led to new correlations based on first principles [132, 124, 9]. All these correlations take the form $\bar{F} = \bar{F}(\text{Re}_p, \phi_s)$, where $\bar{F}$ is the nor-

malized fluid-particle force, Re_p is the particle Reynolds number and ϕ_s is the solid volume fraction of the system. Although recent drag relations seem accurate over a wide range of parameters (e.g. in [124], $Re_p \leq 1000$, $0.1 \leq \phi_s \leq 0.6$), they only provide an average value of the fluid-particle force, irrespective of the local organization of the solid phase. The dynamics of the solid phase is thus somehow filtered as we are missing details about the local forces. Hence, there is a great interest in building models for the fluid force acting on a given particle based on the quantities available at the level of the fluid cell, i.e. Re_p , ϕ_s , and on the organization of the particle's neighborhood. Recent studies addressed this problem. Akiki et al. [2] first tried to correlate the drag and lift forces acting on a spherical particle immersed in an array to some anisotropic measures of its neighborhood. The same authors later proposed a pairwise interaction extended point-particle (PIEP) model [3]. To model the force acting on a particle, the idea is to compute the individual perturbation created by each of its neighbors, superimpose the contributions and use the resulting undisturbed flow (i.e. the flow that would exist in the absence of the particle) into Faxén's law [39] to obtain the different contributions of the fluid force. Their method was then extended to model the torque exerted on a particle [4] and to handle configurations at higher volume fractions [89]. Very recently, Seyed-Ahmadi and Wachs [110] developed a probability-based microstructure-informed point-particle (MPP) model. In their model, the forces and torques acting on a particle are conditioned in order to reveal some patterns in the spatial distribution of the near neighbors. Probability maps are then constructed based on conditional values of forces/torques and further used in a regression model. Their model was shown to be able to predict up to 84 % of the drag force, 78% of the lift force and 86 % of the torque. For time-varying configurations, another type of approach amounts to model the instantaneous fluid force experienced by a particle as a stochastic process [35, 133, 47]. In [35], the stochastic formulation of the drag law proposed by the authors is able to recover the level of particle fluctuations (i.e. the granular temperature) in liquid-solid fluidized beds more correctly than the fully deterministic average drag law formulation.

In this work, we first investigate through PR-DNS the distribution of the fluid force acting on static arrays of randomly dispersed particles. Then, we attempt to link the force experienced by a reference particle to some tensor quantities that characterize the organization of the local microstructure formed by its neighboring particles. Our approach is inspired from the so-called fabric tensor used to predict stresses in granular media [94, 83]. Finally, a simple multi-linear model is proposed to predict the fluid-particle force from microstructure characteristic quantities. The opportunity to add a stochastic contribution to the microstructure-based deterministic model is also

discussed. This study introduces a novel comprehensive physics-based methodology that should lead to improved models for the fluid-particle force.

The chapter is organized as follows. Section 2.2 describes the numerical set-up used in our resolved simulations. Section 2.3 presents our results for the distribution of the fluid force acting on spherical particles immersed in random arrays. The statistics of the force distribution are analyzed at different Reynolds numbers and volume fractions. Section 2.4 introduces the tensor and vector quantities used to characterize the microstructure. Section 2.5 details the search for existing correlations between the fluid force acting on a particle and the tensor quantities used to describe its neighborhood. On this basis, we propose a simple multi-linear model in Section 2.6 whose accuracy is evaluated on independent test cases. Finally, Section 2.7 summarises the main outcomes of this work and provides suggestions for future research.

2.2 Numerical set-up

Let us consider the flow of a fluid with a superficial velocity $\mathbf{U}_0 = U_0 \mathbf{e}_\parallel$ past a monodisperse, homogeneous array of N_p spherical particles of diameter d_p . The solid volume fraction ϕ_s of the array is computed over the volume V of the domain as

$$\phi_s = \frac{1}{V} \int_V \chi_s(\mathbf{x}) d\mathbf{x}, \quad (2.1)$$

where the solid phase indicator function χ_s is defined as

$$\chi_s(\mathbf{x}) = \begin{cases} 1 & \text{if } \mathbf{x} \text{ is in the solid phase,} \\ 0 & \text{otherwise.} \end{cases} \quad (2.2)$$

The particle Reynolds number is classically defined as

$$\text{Re}_p = \frac{(1 - \phi_s) \|\mathbf{u}_f - \mathbf{u}_s\| d_p}{\nu}, \quad (2.3)$$

where $\mathbf{u}_f$ and $\mathbf{u}_s$ are the phase-averaged (or interstitial) velocities of the fluid and the solid phases, respectively. The fluid-phase averaged velocity is linked to the superficial velocity $\mathbf{U}_0$ by the relation

$$\mathbf{u}_f = \frac{\mathbf{U}_0}{(1 - \phi_s)}. \quad (2.4)$$

In the case of a fixed array of particles, $\mathbf{u}_s = 0$, and the Reynolds number simply reads

$$\text{Re}_p = \frac{U_0 d_p}{\nu}. \quad (2.5)$$

The spherical particles are randomly distributed in a tri-periodic box with dimensions $L_x = L_y = 8d_p$ and $L_z = 12d_p$. The mean flow is aligned with the z direction and the flow rate velocity U_0 is prescribed by an external pressure gradient. For statistical convergence reasons, three independent realizations of the flow have been simulated for each value of ϕ_s . The number of particles required in the box is determined as

$$N_p = \frac{\phi_s V_{\text{box}}}{V_p}, \quad (2.6)$$

with $V_{\text{box}} = L_x L_y L_z$ and $V_p = \frac{\pi d_p^3}{6}$.

The simulation domain is depicted in Figure 2.1, with $N_p = 440$ randomly distributed particles and a corresponding solid volume fraction $\phi_s = 0.30$. Three particle Reynolds numbers are considered, $\text{Re}_p = (10, 50, 100)$, and the grid is refined as Re_p is increased. The corresponding grid resolutions are $N_d = \frac{d_p}{h} = (24, 32, 48)$. For each Re_p , the flow is solved at four volume fractions, $\phi_s = (0.10, 0.20, 0.30, 0.40)$. In the following, all statistics have been computed at steady state, over the three independent realizations. To illustrate, Figure 2.2 shows a longitudinal slice of the magnitude of the velocity field for one realization of the flow at $(\text{Re}_p, \phi_s) = (50, 0.30)$.

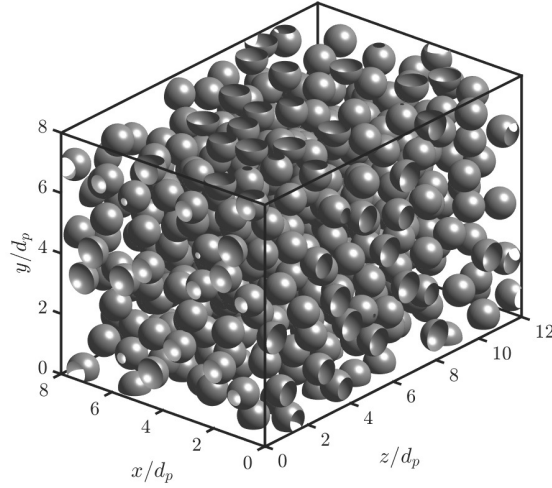


Figure 2.1: Computational domain with a random assembly of spheres, $\phi_s = 0.30$.

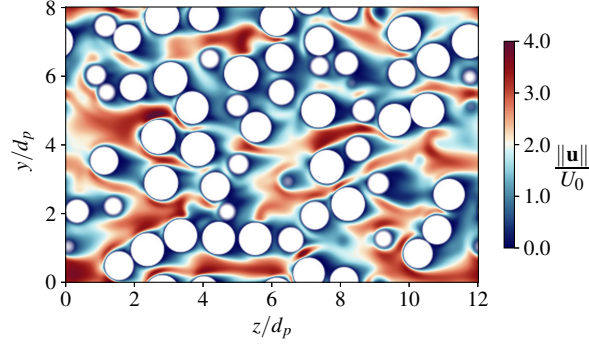


Figure 2.2: Velocity field magnitude in the slice of a realization of the flow past a fixed assembly of spheres at $(\text{Re}_p, \phi_s) = (50, 0.30)$.

2.3 Fluid-particle force in monodisperse random arrays of spheres

2.3.1 Mean fluid-particle force

The force $\mathbf{F}_p$ exerted by the fluid on a given particle can be decomposed into its stream-wise and transverse components as follows,

$$\mathbf{F}_p = F_{p\parallel} \mathbf{e}_{\parallel} + F_{p\perp} \mathbf{e}_{\perp}, \quad (2.7)$$

where $\mathbf{e}_{\perp}$ is a unit vector orthogonal to the mean flow, defined as

$$\mathbf{e}_{\perp} = \frac{\mathbf{F}_p - F_{p\parallel} \mathbf{e}_{\parallel}}{\|\mathbf{F}_p - F_{p\parallel} \mathbf{e}_{\parallel}\|}. \quad (2.8)$$

By construction of Eqs. (2.7) and (2.8), $F_{p\perp}$ is always positive since it corresponds to the norm of the component of the force orthogonal to the mean flow. The decomposition of the fluid-particle force in streamwise and orthogonal components is illustrated in Figure 2.3.

For a random array of particles, the mean fluid-particle force is aligned with the mean flow, i.e.

$$\langle \mathbf{F}_p \rangle = \langle F_{p\parallel} \rangle \mathbf{e}_{\parallel}, \quad (2.9)$$

where

$$\langle \mathbf{F}_p \rangle = \frac{1}{N_p} \sum_{k=1}^{N_p} \mathbf{F}_p^{(k)} \quad (2.10)$$

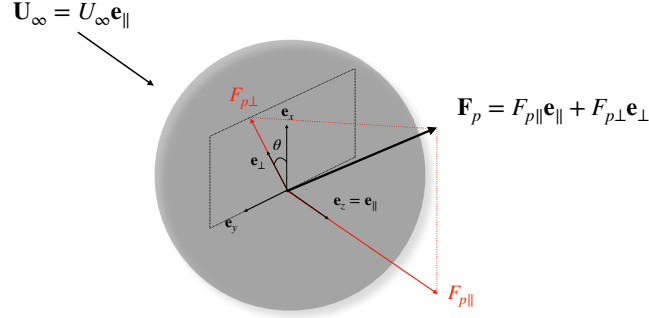


Figure 2.3: Fluid force acting on a spherical particle immersed in a random array: decomposition in streamwise and orthogonal components.

is the average of the total fluid-particle force (here including the mean pressure gradient, see details in Appendix B) over the N_p particles. The normalized mean fluid-particle force is then defined as

$$\bar{F} = \frac{\langle F_{p\parallel} \rangle}{F_{St}}, \quad (2.11)$$

where $F_{St} = 3\pi\mu d_p U_0$ is the drag force acting on an isolated sphere in Stokes regime. Table 2.1 summarizes some commonly used correlations to estimate the normalized mean fluid-particle force as defined by Eq. (2.11).

The force experienced by each particle is computed from the IBM forcing (see Eq. (1.32)) as

$$\mathbf{F}_p = \rho_f \left[- \sum_l \mathbf{F}_l \Delta V_l + \frac{d}{dt} \left(\int_{V_p} \mathbf{u} dV \right) \right], \quad (2.12)$$

where the second term on the right-hand side vanishes at steady-state. We report in Figure 2.4 the values of $\bar{F}$ (average and 95% confidence interval) for all the cases investigated. The curves corresponding to the correlations given in Table 2.1 are also shown. It must be stressed that these results include the contribution of the mean pressure gradient in the fluid force, in contrast to other studies. We note that our data points are globally close to the most recent correlations from Tenneti et al. [132], Beetstra et al. [9] and Tang et al. [124], which were all derived from resolved simulations. We also note that, with only three different realizations, the uncertainty on the mean value

Table 2.1: Literature correlations for the normalized mean fluid-particle force as a function of the Reynolds number, $\text{Re}_p = \frac{U_0 d_p}{\nu}$, and of the solid volume fraction ϕ_s .

Author	Normalized mean fluid-particle force
Ergun [33]	$\bar{F} = \frac{150}{18} \frac{\phi_s}{(1-\phi_s)^3} + \frac{1.75}{18} \frac{\text{Re}_p}{(1-\phi_s)^3}$
Wen and Yu [152]	$\bar{F} = \left(1 + 0.15 \text{Re}_p^{0.687}\right) (1-\phi_s)^{-4.65} = \bar{F}_{WY}$
Tenneti et al. [132]	$\bar{F} = \bar{F}_{WY} (1-\phi_s)^{1.65} + F_1(\phi_s) + F_2(\text{Re}_p, \phi_s)$ $F_1 = 5.81 \frac{\phi_s}{(1-\phi_s)^3} + 0.48 \frac{\phi_s^{1/3}}{(1-\phi_s)^4}$ $F_2 = \phi_s^3 \text{Re}_p \left(0.95 + 0.61 \frac{\phi_s^3}{(1-\phi_s)^2} \right)$
Beetstra et al. [9]	$\bar{F} = 10 \frac{\phi_s}{(1-\phi_s)^3} + (1-\phi_s) \left(1 + 1.5 \sqrt{\phi_s} \right)$ $+ \frac{0.413}{(1-\phi_s)^3} \frac{\text{Re}_p}{24} \left(\frac{(1-\phi_s)^{-1} + 3\phi_s(1-\phi_s) + 8.4 \text{Re}_p^{-0.343}}{1 + 10^3 \phi_s \text{Re}_p^{-(1+4\phi_s)/2}} \right)$
Tang et al. [124]	$\bar{F} = 10 \frac{\phi_s}{(1-\phi_s)^3} + (1-\phi_s) \left(1 + 1.5 \sqrt{\phi_s} \right) + \left[0.11 \phi_s (1 + \phi_s) \right.$ $\left. - \frac{0.00456}{(1-\phi_s)^4} + \left(0.169(1-\phi_s) + \frac{0.0644}{(1-\phi_s)^4} \right) \text{Re}_p^{-0.343} \right] \frac{\text{Re}_p}{(1-\phi_s)}$

is very small (the error bars do not exceed the size of the square symbols), which confirms that the size of the computational domain, combined with the three independent realizations, is sufficient to properly reproduce the statistics of the mean force.

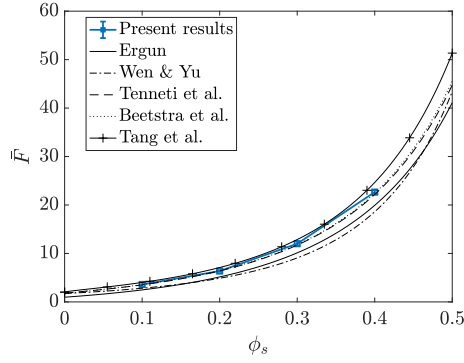
2.3.2 Fluid-particle force distribution

We now aim at characterizing the statistics of the fluid-particle force distribution in the array. The deviation of a quantity X with respect to its average $\langle X \rangle$ is identified by a prime symbol as

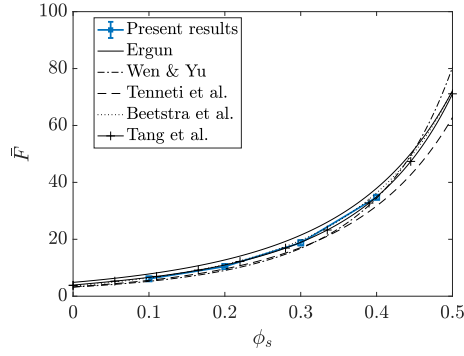
$$X' = X - \langle X \rangle \quad (2.13)$$

and the variance of X is subsequently obtained as

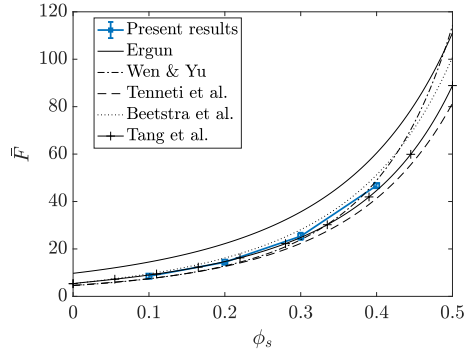
$$\sigma_X^2 = \langle X'^2 \rangle. \quad (2.14)$$



(a)



(b)



(c)

Figure 2.4: Average normalized fluid-particle force at (a) $Re_p = 10$, (b) $Re_p = 50$ and (c) $Re_p = 100$. The error bars indicate the 95% confidence interval on the mean value (they here never exceed the size of the square symbols).

The skewness and kurtosis are respectively defined as

$$S_X = \frac{\langle X'^3 \rangle}{\sigma_X^3} \quad (2.15)$$

and

$$\mathcal{K}_X = \frac{\langle X'^4 \rangle}{\sigma_X^4}. \quad (2.16)$$

These higher order moments allow to assess more precisely the deviation of a probability density function (pdf) from a normal distribution (with theoretical skewness and kurtosis equal to 0 and 3, respectively). The covariance between two variables X and Y is given by

$$\text{cov}(X, Y) = \langle X'Y' \rangle \quad (2.17)$$

and the Pearson correlation coefficient between these two variables is then obtained as

$$\rho_{XY} = \frac{\text{cov}(X, Y)}{\sigma_X \sigma_Y}. \quad (2.18)$$

In our numerical set-up, the mean flow is taken aligned with the z direction, so that $\mathbf{e}_{\parallel} = \mathbf{e}_z$ and $F_{p\parallel} = F_{p,z}$. The transverse component of the fluid force can also be decomposed into its cartesian components: $F_{p\perp}\mathbf{e}_{\perp} = F_{p,x}\mathbf{e}_x + F_{p,y}\mathbf{e}_y$. Since we chose a specific reference frame where the streamwise direction is aligned with one of the main directions, the statistical distributions of any quantity along the two other directions should be identical. Therefore, the statistics of the fluid-particle force are only reported for the z and x components, without loss of generality. Figure 2.5 shows the scatter plots between $F_{p,z}$ and $F_{p,x}$ and between $F_{p,y}$ and $F_{p,x}$ for the case at $\text{Re}_p = 50$ and $\phi_s = 0.30$. They both display a Gaussian shape. It can still be observed in Figure 2.5a that large deviations in the transverse force component tend to be more frequently observed with a larger value of the streamwise force component. However, this effect is tenuous, so that the streamwise and transverse components of the force will be modeled independently in the following.

The pdf's of $F_{p,z}$ and $F_{p,x}$ for the cases at $\text{Re}_p = 50$ are shown in Figure 2.6, for all volume fractions. Estimates for the different statistics of the force are reported in Table 2.2. The fluctuations of the streamwise component of the force oscillate between 24 and 30 % of its mean value and the standard deviation seems to increase slightly with Re_p and to decrease with the volume fraction, as previously reported by Akiki et al. [2]. The estimates for the skewness are close to zero, although always positive, while the kurtosis takes values around 3, confirming the quasi-normal distribution of $F_{p,z}$ identified in Figure 2.6. Hence, the streamwise component of the force reads

$F_{p,z} \sim \mathcal{N}(\langle F_{p,z} \rangle, \sigma_{F_{p,z}})$, where the notation $X \sim \mathcal{N}(\mu, \sigma)$ indicates that the random variable X follows a normal distribution of expected value μ and standard deviation σ . The slight left-skewness of the pdf of $F_{p,z}$ ($S_{F_{p,z}} > 0$) might be explained as follows. A particle immersed in a random array can hardly be in a configuration such that the streamwise component of the fluid force becomes negative, i.e. opposite to the mean flow. Conversely, situations may occur where a particle is quite isolated in the array, facing the upstream flow with no shielding effect. Then, the streamwise component of the fluid force acting on this particle can exceed twice its mean value, as observed on the right tail of Figure 2.6a.

Regarding the transverse component $F_{p,x}$ of the fluid force, its distribution is centered around 0, as expected, and the standard deviation amounts to 15 to 18% of the mean streamwise fluid force. The skewness and kurtosis of $F_{p,x}$ also take values close to 0 and 3, which validates the normal distribution approximation, i.e. $F_{p,x} \sim \mathcal{N}(0, \sigma_{F_{p,x}})$. The norm of the transverse component of the fluid force can be expressed in terms of the transverse cartesian components as $F_{p\perp} = \sqrt{F_{p,x}^2 + F_{p,y}^2} \geq 0$. Since $F_{p,x}$ and $F_{p,y}$ follow the same normal distribution with zero mean, $F_{p\perp}$ follows a Rayleigh distribution with scale parameter $\sigma_{F_{p,x}} = \sigma_{F_{p,y}}$ ¹, which reads $F_{p\perp} \sim \text{Rayleigh}(\sigma_{F_{p,x}})$. The histogram representing the effective distribution of $F_{p\perp}$ at different volume fractions is compared to the Rayleigh distribution computed with $\sigma_{F_{p,x}}$ in Figure 2.7. The quality of the fit increases with the solid volume fraction, probably due to the increased statistical convergence given the larger number of particles. Finally, the unit vector $\mathbf{e}_\perp$ can be defined by the angle θ formed with the x axis in the xy plane (see scheme in Figure 2.3), i.e. $\mathbf{e}_\perp = \cos(\theta)\mathbf{e}_x + \sin(\theta)\mathbf{e}_y$. Since $F_{p,x}$ and $F_{p,y}$ are uncorrelated and have zero mean, θ is uniformly distributed between 0 and 2π , which reads $\theta \sim \mathcal{U}([0, 2\pi])$.

As a result, the fluctuation $\mathbf{F}'_p$ of the force can be statistically modeled by an anisotropic Gaussian distribution ($\sigma_{F_{p,x}} = \sigma_{F_{p,y}} \leq \sigma_{F_{p,z}}$). However, with such a model, two neighboring particles will experience uncorrelated fluid forces, which is inconsistent with the physical observations. The purpose of the next section is therefore to unveil the dependence of the fluid force experienced by a particle on certain properties of the microstructure formed by its neighboring particles.

¹Equivalently, $\frac{F_{p\perp}^2}{\sigma_{F_{p,x}}^2}$ follows a chi-square distribution with two degrees of freedom.

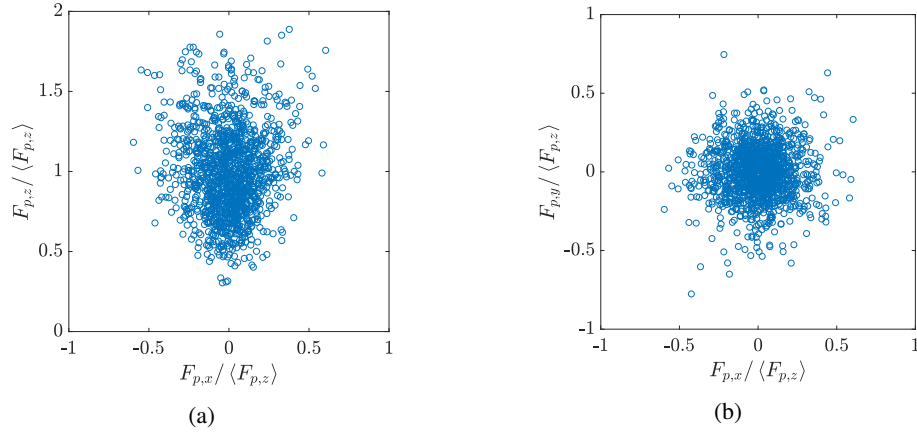


Figure 2.5: Scatter plots between (a) the streamwise and one transverse component of the force and (b) the two transverse components of the force for the case at $(\text{Re}_p, \phi_s) = (50, 0.3)$.

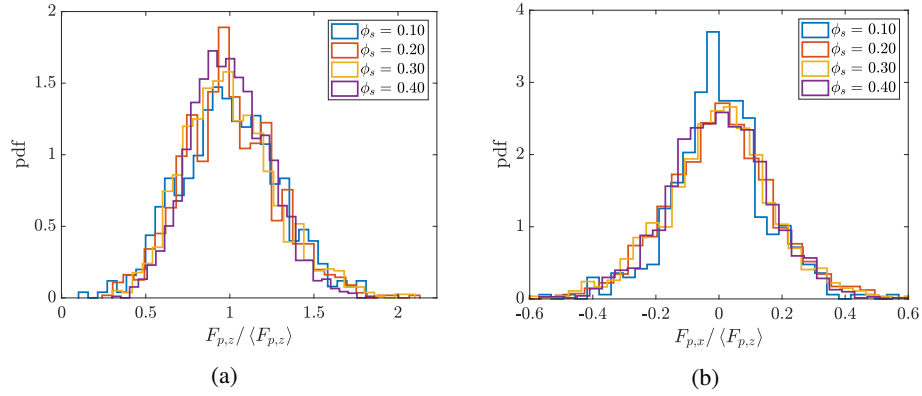


Figure 2.6: Distribution of (a) the streamwise and (b) the transverse components of the fluid force for the cases at $\text{Re}_p = 50$.

Table 2.2: Statistics of the streamwise (z) and transverse (x) components of the fluid force.

ϕ_s	$\frac{\langle F_{p,z} \rangle}{F_{St}}$	$\frac{\sigma_{F_{p,z}}}{\langle F_{p,z} \rangle}$	$S_{F_{p,z}}$	$\mathcal{K}_{F_{p,z}}$	$\frac{\langle F_{p,x} \rangle}{\langle F_{p,z} \rangle}$	$\frac{\sigma_{F_{p,x}}}{\langle F_{p,z} \rangle}$	$S_{F_{p,x}}$	$\mathcal{K}_{F_{p,x}}$
$Re_p = 10$								
0.10	3.59	0.26	0.28	3.05	5×10^{-5}	0.15	-0.04	3.04
0.20	6.37	0.25	0.39	3.13	-5×10^{-6}	0.16	-0.20	3.61
0.30	12.00	0.25	0.48	3.31	4×10^{-6}	0.17	-0.04	3.35
0.40	22.64	0.20	0.28	2.94	2×10^{-6}	0.16	-0.05	3.19
$Re_p = 50$								
0.10	6.12	0.29	0.06	2.82	9×10^{-4}	0.15	-0.07	4.10
0.20	10.43	0.28	0.29	3.23	3×10^{-5}	0.17	-0.23	4.10
0.30	18.75	0.28	0.51	3.40	-4×10^{-6}	0.17	-0.04	3.53
0.40	34.75	0.24	0.24	2.92	5×10^{-6}	0.16	-0.02	3.25
$Re_p = 100$								
0.10	8.51	0.30	0.03	3.00	4×10^{-5}	0.15	0.13	4.54
0.20	14.41	0.28	0.28	3.38	-4×10^{-5}	0.18	-0.27	4.61
0.30	25.25	0.29	0.50	3.45	1×10^{-7}	0.18	0.05	3.56
0.40	46.71	0.25	0.22	2.87	2×10^{-6}	0.17	-0.02	3.30

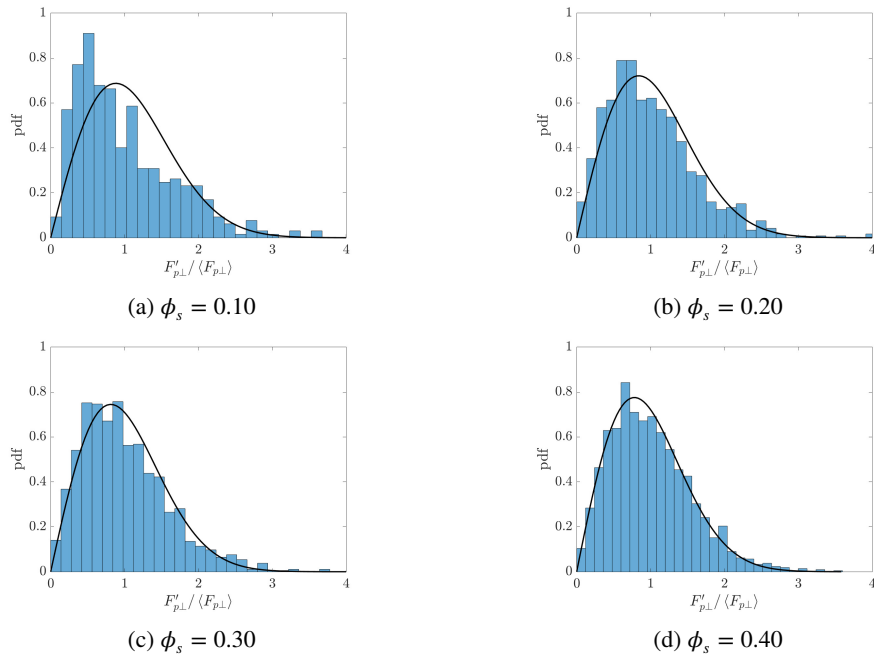


Figure 2.7: Distribution of the norm of the transverse component of the fluid force for the cases at $\text{Re}_p = 50$, and the corresponding Rayleigh distribution with scale parameter $\sigma_{F_{p,x}}$ (—).

2.4 Microstructure characterization

2.4.1 Orientation tensors and invariants

Let us consider a particle immersed in a randomly distributed array such as presented above. From dimensional analysis, the force applied by the fluid on this particle can be expressed in very general terms as

$$\frac{\mathbf{F}_p}{F_{St}} = \bar{\mathbf{F}}_p \left(\text{Re}_p, \phi_s, \mathbf{e}_{\parallel}, \frac{\{\mathbf{r}_q\}}{d_p} \right), \quad (2.19)$$

where $\bar{\mathbf{F}}_p$ is a dimensionless function and $\{\mathbf{r}_q\} = \mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N$ represents the positions of the N neighboring particles with respect to the reference particle. The expression given by Eq. (2.19) is very general, but it would be extremely complex to model the combined action of all the neighbors on the force experienced by the particle. However, the full set of neighbor positions $\{\mathbf{r}_q\}$ can probably be approximated by a limited number of quantities that characterize the microstructure formed by the distribution of the near neighbors in space. It is then proposed to define a set of tensor quantities inspired from the fabric tensor used to predict stresses in granular media [94, 83, 71, 72]. In that community, the fabric tensor is a global quantity that characterizes the organization (level of anisotropy and main orientation) of an ensemble of grains or a distribution of voids, e.g. in sand or rock materials. By analogy, a *local* second-order fabric tensor is introduced to characterize the neighborhood of a given particle. It is defined as

$$H_{p,ij} = \frac{1}{N_b} \sum_{q=1}^{N_b} w_q n_{q,i} n_{q,j}, \quad (2.20)$$

where N_b is the number of neighbors taken into account, $\mathbf{n}_q = \frac{\mathbf{r}_q}{\|\mathbf{r}_q\|}$ is the unit vector joining the center of the particle to that of its q th nearest neighbor and w_q is the weight attributed to that neighbor. The trace of $\mathbf{H}_p$ gives the average value of the weight assigned to the N_b neighbors. Indeed, we have that

$$\text{tr}(\mathbf{H}_p) = H_{p,kk} = \frac{1}{N_b} \sum_{q=1}^{N_b} w_q, \quad (2.21)$$

where the Einstein's summation convention is used. As the relative influence of a neighbor particle shall decrease with its distance to the reference particle, it is proposed to use as weight function a Gaussian filter, i.e.

$$w_q = w(\|\mathbf{r}_q\|) = \exp \left(- \left(\frac{\|\mathbf{r}_q\|}{\sigma_0} \right)^2 \right), \quad (2.22)$$

with σ_0 , its characteristic width. In general, the value taken by σ_0 should depend on both the volume fraction ϕ_s and the flow regime (i.e. Re_p). As noted by Seyed-Ahmadi and Wachs [110], distant neighbors shall contribute more in viscous regimes due to the elliptic nature of the governing equations. In a random array, the mean distance to the first neighbor is known to decrease with the solid fraction proportionally to $\phi_s^{-1/3}$. Therefore, it is proposed to express σ_0 as

$$\sigma_0 = c(\text{Re}_p) \frac{d_p}{\phi_s^{1/3}}, \quad (2.23)$$

where c is at most a function of the particle Reynolds number. The way we determined c is discussed later. From $\mathbf{H}_p$, one defines the traceless tensor $\mathbf{G}_p$ as

$$G_{p,ij} = \frac{H_{p,ij}}{H_{p,kk}} - \frac{\delta_{ij}}{3} = \frac{\sum_{q=1}^{N_b} w_q n_{q,i} n_{q,j}}{\sum_{q=1}^{N_b} w_q} - \frac{\delta_{ij}}{3}, \quad (2.24)$$

which amounts to the deviatoric part of $\mathbf{H}_p$ normalized by its trace. As discussed in previous works [71, 72], the trace of the fabric tensor reflects its isotropic part, which is here related to the local porosity around the particle, while $\mathbf{G}_p$ measures the anisotropy of the local microstructure.

A normalized first-order tensor (i.e. vector) $\mathbf{K}_p$ is built in a similar way as

$$K_{p,i} = \frac{\sum_{q=1}^{N_b} w_q n_{q,i}}{\sum_{q=1}^{N_b} w_q}. \quad (2.25)$$

Since $\mathbf{G}_p$ is a second order even tensor, reversing the axes of the reference frame will keep it unchanged. In other words, $\mathbf{G}_p$ is not able to differentiate between two identical microstructures by point reflection through the center of the reference particle. Instead, it provides information about the local alignment of the microstructure. Conversely, $\mathbf{K}_p$ is odd and point reflection will result in a change of sign. Complementary to $\mathbf{G}_p$, $\mathbf{K}_p$ indicates the main direction of the microstructure orientation. Higher-order tensors can be constructed in the same fashion. Yet, as a first step and in order to remain as simple as possible, the microstructure will here be characterized using zero, first and second order tensors. Hence, Eq. (2.19) is recast as

$$\frac{\mathbf{F}_p}{F_{St}} = \bar{\mathbf{F}}_p^{(m)}(\text{Re}_p, \phi_s, \mathbf{e}_{\parallel}, \text{tr}(\mathbf{H}_p), \mathbf{K}_p, \mathbf{G}_p) + \delta \bar{\mathbf{F}}_p, \quad (2.26)$$

where the superscript (m) indicates the part of $\bar{\mathbf{F}}_p$ captured by the microstructure-based model and $\delta \bar{\mathbf{F}}_p$ is the (normalized) random part, i.e. the deviation between the measured force and the value returned by the model. It is further assumed that $\delta \bar{\mathbf{F}}_p$ is

uncorrelated with the microstructure quantities retained in the model. Current relations for the mean drag force only consider the first three variables in the expression of $\bar{\mathbf{F}}_p^{(m)}$, i.e. the Reynolds number, the volume fraction and the direction of the mean flow.

Some invariants are now defined from the tensor quantities introduced above. We first consider isotropic invariants that do not involve the mean flow direction. The principal invariant of $\mathbf{K}_p$ is its norm, defined as $\|\mathbf{K}_p\| = (K_{p,i}K_{p,i})^{1/2}$. For the second-order tensor $\mathbf{G}_p$, we define the following isotropic invariants,

$$I_{\mathbf{G}_p,1} = \text{tr}(\mathbf{G}_p) = 0 \text{ by definition,} \quad (2.27a)$$

$$I_{\mathbf{G}_p,2} = \|\mathbf{G}_p\| = (G_{p,ij}G_{p,ji})^{1/2}, \quad (2.27b)$$

$$I_{\mathbf{G}_p,3} = \det(\mathbf{G}_p). \quad (2.27c)$$

These quantities do not contain information on the direction of the flow and their ability to model the fluid force should be small. Hence, we introduce new invariants built from $\mathbf{K}_p$, $\mathbf{G}_p$ and the flow direction direction $\mathbf{e}_\parallel$. The vector $\mathbf{K}_p$ is decomposed into its streamwise and transverse components as

$$\mathbf{K}_p = K_{p\parallel}\mathbf{e}_\parallel + K_{p\perp}\mathbf{e}_\perp^*, \quad (2.28)$$

where $K_{p\parallel}$ and $K_{p\perp}$ are scalar invariants and the orthogonal direction vector $\mathbf{e}_\perp^*$ is given by

$$\mathbf{e}_\perp^* = \frac{\mathbf{K}_p - K_{p\parallel}\mathbf{e}_\parallel}{\|\mathbf{K}_p - K_{p\parallel}\mathbf{e}_\parallel\|}. \quad (2.29)$$

It must be stressed that, although $\mathbf{e}_\perp$ and $\mathbf{e}_\perp^*$ are two unit vectors perpendicular to the mean flow direction, they are a priori not aligned.

We now define the normalized vector β_p by taking the scalar product between $\mathbf{G}_p$ and the flow direction $\mathbf{e}_\parallel$:

$$\beta_p = \mathbf{G}_p \cdot \mathbf{e}_\parallel. \quad (2.30)$$

Similar to $\mathbf{K}_p$, β_p is decomposed into streamwise and transverse components as

$$\beta_p = \beta_{p\parallel}\mathbf{e}_\parallel + \beta_{p\perp}\mathbf{e}_\perp^{**} \quad (2.31)$$

and $\mathbf{e}_\perp^{**}$ is given by

$$\mathbf{e}_\perp^{**} = \frac{\beta_p - \beta_{p\parallel}\mathbf{e}_\parallel}{\|\beta_p - \beta_{p\parallel}\mathbf{e}_\parallel\|}. \quad (2.32)$$

Given the anisotropic nature of the fluid force, the components of $\mathbf{K}_p$ and β_p should be better candidates as predictive variables compared to the isotropic invariants defined earlier.

2.4.2 Model parameters

To close the theory developed in the previous section, some parameter values need to be fixed. First, the number N_b of neighbors taken into account in the definition of $\mathbf{H}_p$ and $\mathbf{K}_p$ must be defined. In their PIEP model, Akiki et al. [3] used 15-40 neighbors to model the streamwise component of the force, while Seyed-Ahmadi and Wachs [110] concluded that using about 20 neighbors was adequate for their MPP model. In the present methodology, the contribution of distant neighbors is gradually reduced by the weight function. Therefore, the values taken by the different quantities built from $\mathbf{K}_p$ and $\mathbf{H}_p$ should converge as N_b increases. The number of neighbors kept in the summation can be related to a normalized cutoff distance R'_c defined as

$$R'_c = R_c \frac{\phi_s^{1/3}}{d_p}, \quad (2.33)$$

where R_c is the distance to the particle center from which particles are discarded from the calculation. Moore et al. [89] derived the link between the number of neighbors taken into account and the cutoff distance. The derivation is reproduced below. If we consider a spherical shell of volume dV located at a distance r from the reference particle, the number of neighbor dN in this shell can be written as

$$dN(r) = g(r, \phi_s) n_v dV, \quad (2.34)$$

where $g(r, \phi_s)$ is the radial distribution function for a given volume fraction ϕ_s and n_v is the particle number density. Since $n_v = \frac{\phi_s}{V_p} = \frac{6\phi_s}{\pi d_p^3}$ and $dV = 4\pi r^2 dr$, and by further assuming that $g(r, \phi_s) = 1$, we have that

$$dN(r) \simeq 24 \frac{\phi_s}{d_p^3} r^2 dr. \quad (2.35)$$

The number of neighbors N_b included in the sphere of radius R_c is obtained by integrating Eq. (2.35) from $r = d_p$ (the smallest possible distance) to $r = R_c$, which gives

$$N_b \simeq 8\phi_s \left(\left(\frac{R_c}{d_p} \right)^3 - 1 \right) = 8 (R_c'^3 - \phi_s). \quad (2.36)$$

As stressed by Moore et al. [89], the approximation that the radial distribution function is equal to one is only valid far from the particle (large r) or at low volume fraction. When this is not the case, the actual number of particles included in the sphere of radius R_c might significantly differ from Eq. (2.36). Given the definitions of σ_0 (Eq. (2.23))

and R'_c (Eq. (2.33)), we have that $\frac{R_c}{\sigma_0} = \frac{R'_c}{c}$. Hence, R'_c will be fixed based on the value chosen for c and the desired ratio between the cutoff distance R_c and the Gaussian filter width σ_0 .

To fix those two parameters, we evaluate the coefficient of determination R^2 of the model proposed in Section 2.6 for the case at $(\text{Re}_p, \phi_s) = (50, 0.30)$ using a range of values for c and for the ratio R_c/σ_0 . It can be observed in Figure 2.8 that the model converges properly beyond $R_c/\sigma_0 = 3$ and that the largest value of R^2 is achieved for $c = 1$. In the following, we will thus use $c = 1$ and a normalized cutoff distance $R'_c = 3$, which corresponds to $N_b \simeq 8R_c'^3 = 216$ neighbors. Actually, it appears from Figure 2.8 that using $R'_c = 2$ (i.e. approximately 64 neighbors) could yield similarly satisfying results while being more tractable in a CFD-DEM approach.

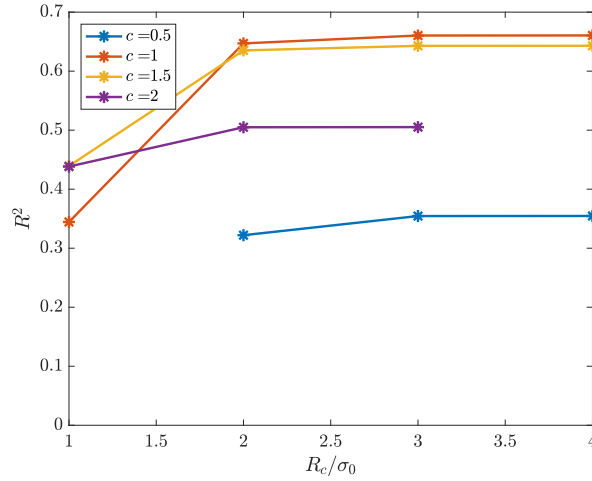


Figure 2.8: Convergence of the coefficient of determination R^2 of the deterministic microstructure-based model as a function of R_c/σ_0 for the case at $(\text{Re}_p, \phi_s) = (50, 0.30)$.

2.4.3 Statistical analysis

Before investigating the possible correlations with the fluid-particle force, the statistics of the microstructure characteristic quantities defined above are analyzed on random assemblies of particles at different volume fractions. First, the alleged link between the trace of $\mathbf{H}_p$ and the local porosity around the reference particle is verified. The topological concept that best describes the space available for a given particle is given

by the Voronoi diagram, which partitions the domain into cells containing the points in space closer to the reference particle than to any other. In Figure 2.9, the Voronoi diagram is built for the random array pictured in Figure 2.1. The volume V_c of the cell associated with each particle can be extracted from the diagram and then used to define the local solid fraction as $\phi_{s,\text{loc}} = \frac{V_p}{V_c}$. The distribution of $\phi_{s,\text{loc}}$ over the

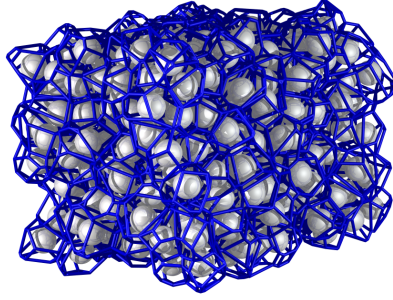


Figure 2.9: Voronoi diagram of a random assembly of particles ($N_p = 440$) with $\phi_s = 0.30$.

ensemble of particles and for various macro-scale solid volume fractions is shown in Figure 2.10. It can be observed that the shape of the pdf is slightly right-skewed in dilute regimes ($\phi_s = 0.1, 0.2$), as the local volume fraction is bounded by 0 on the left, while it resembles more a normal distribution in denser regimes. Figure 2.11 shows the distribution of $\text{tr}(\mathbf{H}_p)$ at different ϕ_s . The scatter plots between $\phi_{s,\text{loc}}$ and $\text{tr}(\mathbf{H}_p)$ in Figure 2.12 confirm that these two quantities are partly correlated, with the coefficient of determination R^2 associated to the linear regression ranging from 0.52 to 0.59.

Figures 2.13 and 2.14 show the distributions of the norm of $\mathbf{K}_p$ and $\mathbf{G}_p$, respectively. In both cases, the mean value of the distribution decreases with ϕ_s , which indicates that dense assemblies are intrinsically more isotropic as they approach close packing. Finally, we note that the determinant of $\mathbf{G}_p$ has an extremely narrow distribution centered around zero (not shown here); it hence provides little information and is discarded for future model development.

Let us now focus on the tensor quantities that were built using the information of the main flow direction. Since $\mathbf{e}_{\parallel} = \mathbf{e}_z$ in our set-up, we have that $K_{p\parallel} = K_{p,z}$, $\beta_{p\parallel} = \beta_{p,z}$ and the transverse components of the vectors $\mathbf{K}_p$ and $\boldsymbol{\beta}_p$ can be expressed in terms of their cartesian components along the x and y directions in the plane orthogonal to the mean flow, i.e. $K_{p\perp}\mathbf{e}_{\perp}^* = K_{p,x}\mathbf{e}_x + K_{p,y}\mathbf{e}_y$ and $\beta_{p\perp}\mathbf{e}_{\perp}^{**} = \beta_{p,x}\mathbf{e}_x + \beta_{p,y}\mathbf{e}_y$. In Figure 2.15, the pdf's of $K_{p,x}$ and $K_{p,z}$ take the form of a normal distribution centered around zero.

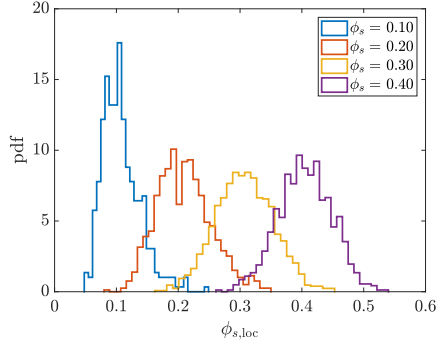


Figure 2.10: Distribution of the local solid volume fraction.

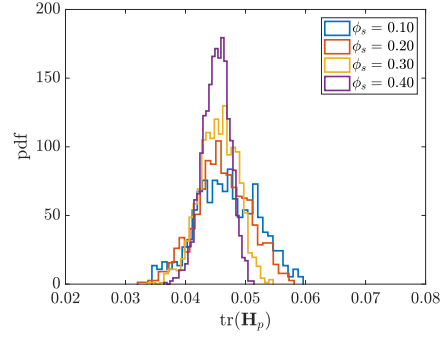


Figure 2.11: Distribution of the trace of $\mathbf{H}_p$.

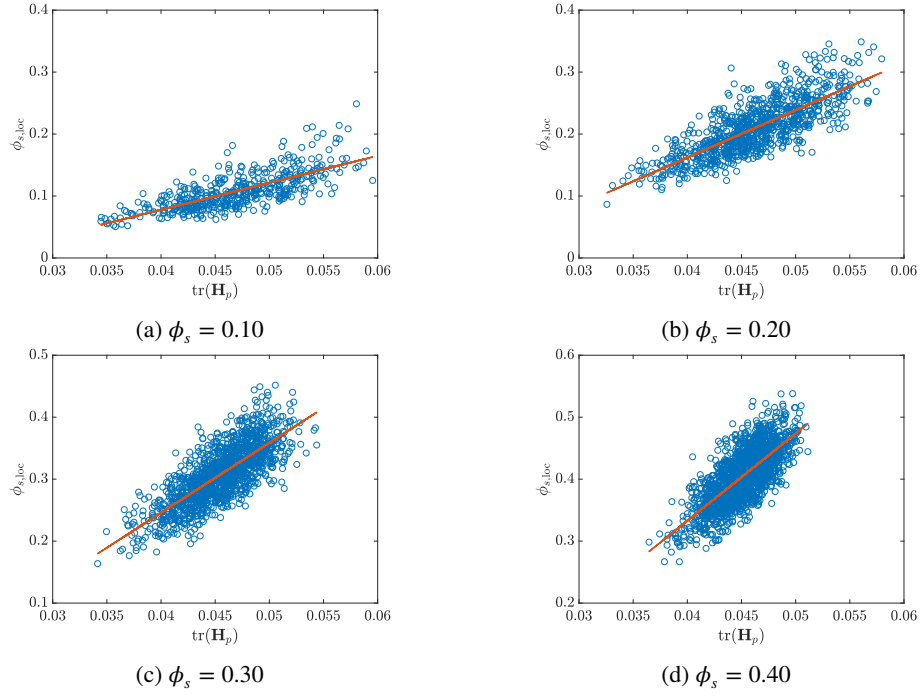
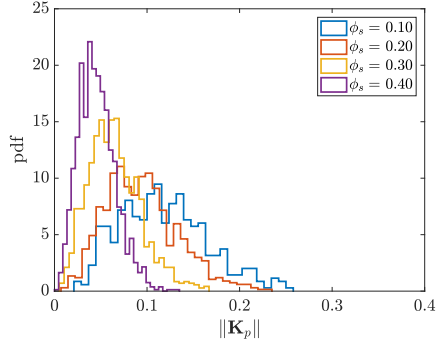
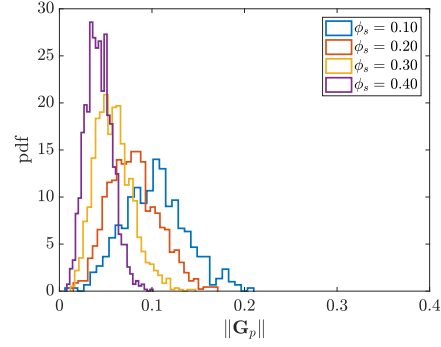


Figure 2.12: Scatter plots and least squares linear regression between $\text{tr}(\mathbf{H}_p)$ and $\phi_{s,loc}$.

The statistics of $K_{p,z}$ and $K_{p,x}$ are gathered in Table 2.3, with similar values for the two components. This observation confirms that the particle arrays are isotropic, with no preferential direction. It can however be observed that the standard deviations of

Figure 2.13: Distribution of the norm of $\mathbf{K}_p$.Figure 2.14: Distribution of the norm of $\mathbf{G}_p$.

$K_{p,z}$ and $K_{p,x}$ decrease with the solid volume fraction. It is thus more likely to have a microstructure that is locally oriented (i.e. anisotropic) in dilute regimes, as previously stated based on the mean values of $\|\mathbf{K}_p\|$ and $\|\mathbf{G}_p\|$. As expected, the skewness and kurtosis take values close to 0 and 3, respectively. Figure 2.16 shows the distributions of $\beta_{p,z}$ and $\beta_{p,x}$. Similar to $\mathbf{K}_p$, their pdf's are centered around zero with a larger spread in dilute regimes. These observations are also supported by the statistics gathered in Table 2.4. Both $\sigma_{\beta_{p,z}}$ and $\sigma_{\beta_{p,x}}$ decrease with ϕ_s , while the skewness and the kurtosis are close to 0 and 3, in all regimes. The statistics of $\beta_{p,x}$ and $\beta_{p,z}$ are similar but, at a given volume fraction, $\sigma_{\beta_{p,x}}$ is always slightly smaller than $\sigma_{\beta_{p,z}}$, which can also be inferred from Figure 2.16. Conversely to $\mathbf{K}_p$, there is no indication that the streamwise and transverse components of β_p should have similar statistics since the information of the mean flow direction, here given by $\mathbf{e}_z$, has already been introduced in the definition of β_p .

In the perspective of future model development, it is important to assess the independence between the variables which may characterize the microstructure. To that end, we provide in Section 2.8.1 the scatter plots between different tensor quantities at volume fractions $\phi_s = 0.30$ (Figure 2.33) and $\phi_s = 0.10$ (Figure 2.34). Their analysis leads to the following conclusions:

- The streamwise and transverse components of $\mathbf{K}_p$ are uncorrelated
- The streamwise and transverse components of β_p are uncorrelated
- $\mathbf{K}_p$ and β_p are uncorrelated
- $\text{tr}(\mathbf{H}_p)$ and $\mathbf{K}_p$ are uncorrelated

- $\text{tr}(\mathbf{H}_p)$ and β_p might be very slightly correlated at low volume fractions.

The same observations are made using the other transverse component (i.e along the y direction) of the vectors $\mathbf{K}_p$ and β_p . Hence, β_p and $\mathbf{K}_p$ can be used as independent predictive variables to model the fluid force acting on a given particle. Whether it is relevant or not to keep the trace of $\mathbf{H}_p$ in the model is discussed in the next section.

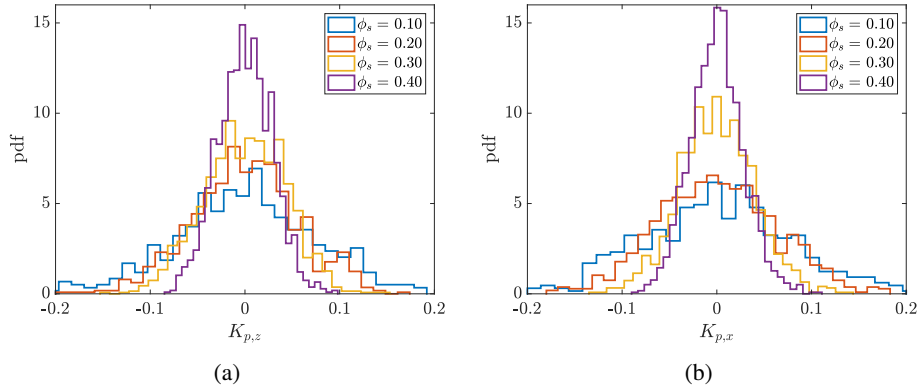


Figure 2.15: Distribution of (a) the streamwise and (b) the transverse components of $\mathbf{K}_p$.

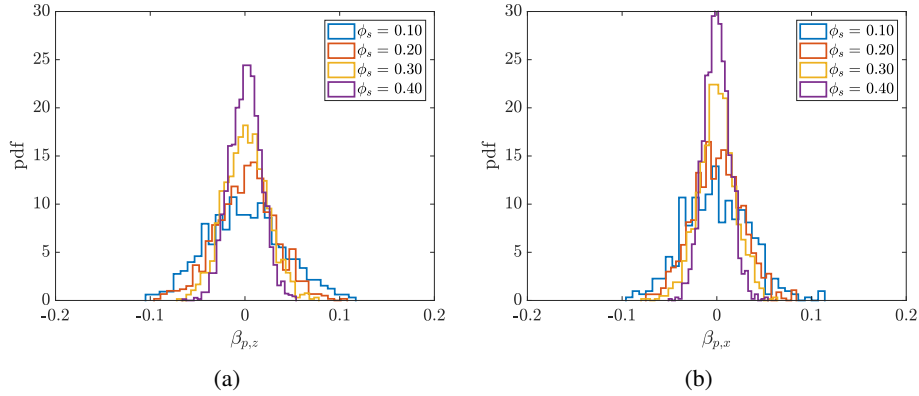


Figure 2.16: Distribution of (a) the streamwise and (b) the transverse components of β_p .

Table 2.3: Statistics of the streamwise and transverse components of $\mathbf{K}_p$

ϕ_s	$\sigma_{K_{p,z}}$	$S_{K_{p,z}}$	$\mathcal{K}_{K_{p,z}}$	$\sigma_{K_{p,x}}$	$S_{K_{p,x}}$	$\mathcal{K}_{K_{p,x}}$
0.10	7.93×10^{-2}	-0.08	2.89	7.82×10^{-2}	-0.03	2.90
0.20	5.59×10^{-2}	-0.12	3.15	6.20×10^{-2}	0.06	2.86
0.30	4.29×10^{-2}	-0.08	2.85	3.97×10^{-2}	0.04	3.29
0.40	2.84×10^{-2}	0.03	2.90	2.79×10^{-2}	0.16	3.22

Table 2.4: Statistics of the streamwise and transverse components of β_p

ϕ_s	$\sigma_{\beta_{p,z}}$	$S_{\beta_{p,z}}$	$\mathcal{K}_{\beta_{p,z}}$	$\sigma_{\beta_{p,x}}$	$S_{\beta_{p,x}}$	$\mathcal{K}_{\beta_{p,x}}$
0.10	4.11×10^{-2}	0.14	2.74	3.43×10^{-2}	0.18	3.14
0.20	3.12×10^{-2}	-0.08	3.12	2.64×10^{-2}	0.07	2.99
0.30	2.27×10^{-2}	0.08	3.02	1.93×10^{-2}	-0.13	3.38
0.40	1.67×10^{-2}	-0.02	3.02	1.37×10^{-2}	0.08	3.19

2.5 Correlation between the fluid-particle force and microstructure characteristic quantities

2.5.1 Streamwise force component

Based on previous observations, we now try to correlate the force exerted by the fluid on a particle with the microstructure characteristic quantities, starting from Eq. (2.26). Figure 2.17 shows the scatter plots between the streamwise force component $F_{p,z}$ and $\text{tr}(\mathbf{H}_p)$, which we showed to be related to the local solid volume fraction. The correlation turns out to be weak. Previous studies [2, 110] also noted that, although the mean fluid force is highly dependent on the macro-scale void fraction, the local value of the porosity does not correlate well with the drag force acting on an individual particle. The same observation is made for the transverse force component (not shown here). Given the limited information provided by $\text{tr}(\mathbf{H}_p)$, it was therefore decided to remove it from the model.

In Figure 2.18, scatter plots between $F_{p,z}$ and $K_{p,z}$ at $\text{Re}_p = 50$ suggest that the streamwise components of $\mathbf{F}_p$ and $\mathbf{K}_p$ are only slightly correlated. Although small, the slope of the regression line is always positive. Indeed, when $K_{p,z}$ takes negative values, the neighborhood of the particle is globally oriented upstream and the shielding effect is more pronounced, resulting in a decrease of the drag force. On the other hand, the scatter plots between $F_{p,z}$ and $K_{p,x}$ in Figure 2.19 show that these two quantities are uncorrelated. The same behavior is observed between $F_{p,z}$ and $K_{p,y}$ (not shown

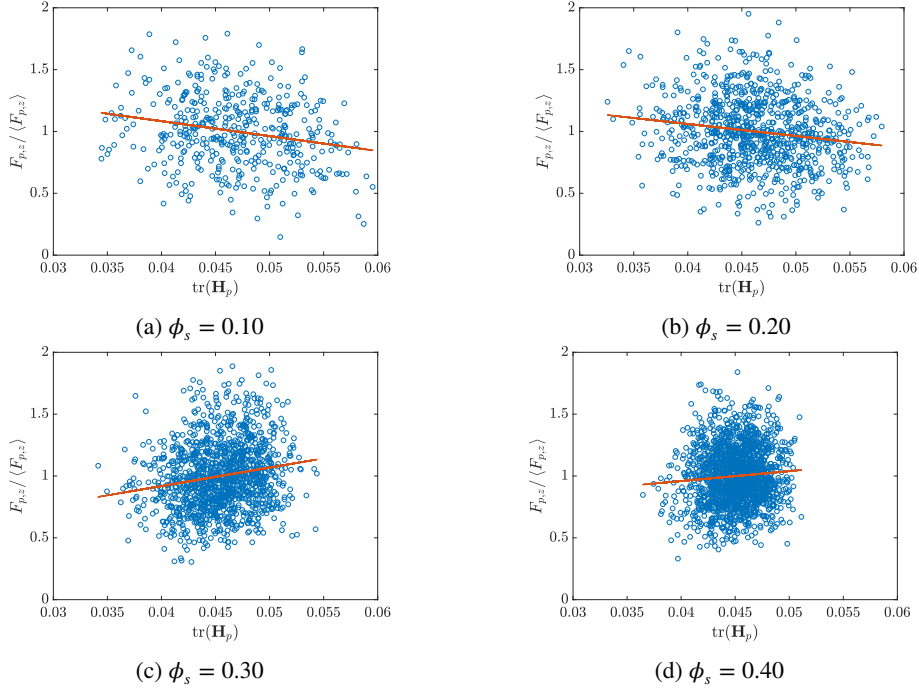


Figure 2.17: Scatter plots and least squares linear regression between $\text{tr}(\mathbf{H}_p)$ and $F_{p,z}$ for the cases at $\text{Re}_p = 50$.

here), which shows that the streamwise component of the force is independent of the transverse components of $\mathbf{K}_p$.

As evidenced by the scatter plots in Figure 2.20, the correlation between $F_{p,z}$ and $\beta_{p,z}$ is much more pronounced. The regression line has a negative slope because positive values of $\beta_{p,z}$ indicate that the neighborhood of the particle is locally aligned with the direction of the flow, hence reducing the drag force. Finally, Figure 2.21 shows that $\beta_{p,x}$ and $F_{p,z}$ are uncorrelated. Again, the same observation is made using the other transverse component (i.e. $\beta_{p,y}$) and for all the Reynolds numbers and volume fractions investigated. It can thus be considered that the transverse components of β_p do not contribute to the variations of the streamwise component of the force.

Table 2.5 reports the square of the correlation coefficient defined by Eq. (2.18) between the streamwise component of the force and the streamwise components of β_p and $\mathbf{K}_p$, for the regimes investigated. The last row contains the sum of the two first rows and corresponds to the theoretical coefficient of determination R^2 of the global

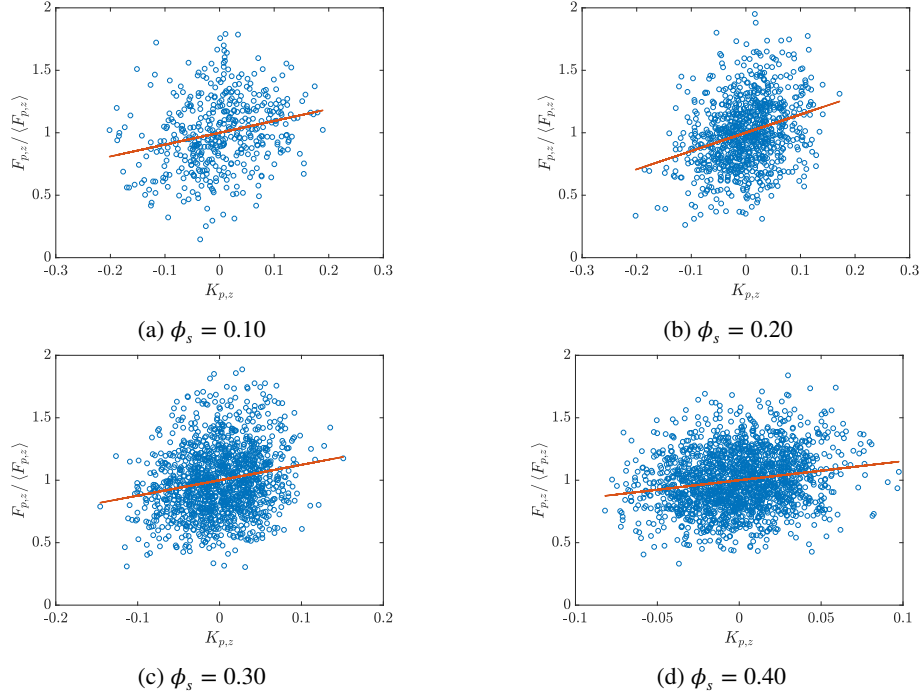


Figure 2.18: Scatter plots and least squares linear regression between $K_{p,z}$ and $F_{p,z}$ for the cases at $\text{Re}_p = 50$.

model as explained later. As deduced from the scatter plots, the strongest correlation is found between $F_{p,z}$ and $\beta_{p,z}$. The corresponding value of ρ^2 increases with ϕ_s while it decreases with Re_p . Indeed, in viscous flows and dense regimes, the flow around the immersed particles display increased fore-aft symmetry. As detailed in Section 2.4, β_p is defined from the even tensor $\mathbf{G}_p$, and, as a result, two mirror microstructures along the streamwise direction will yield the same value for $\beta_{p,z}$. It is therefore not surprising that $\beta_{p,z}$ performs better in regimes showing increased symmetry. The contribution of $K_{p,z}$ to the variation of $F_{p,z}$ is much more tenuous but it appears to increase slightly with the Reynolds number and decrease with the solid fraction.

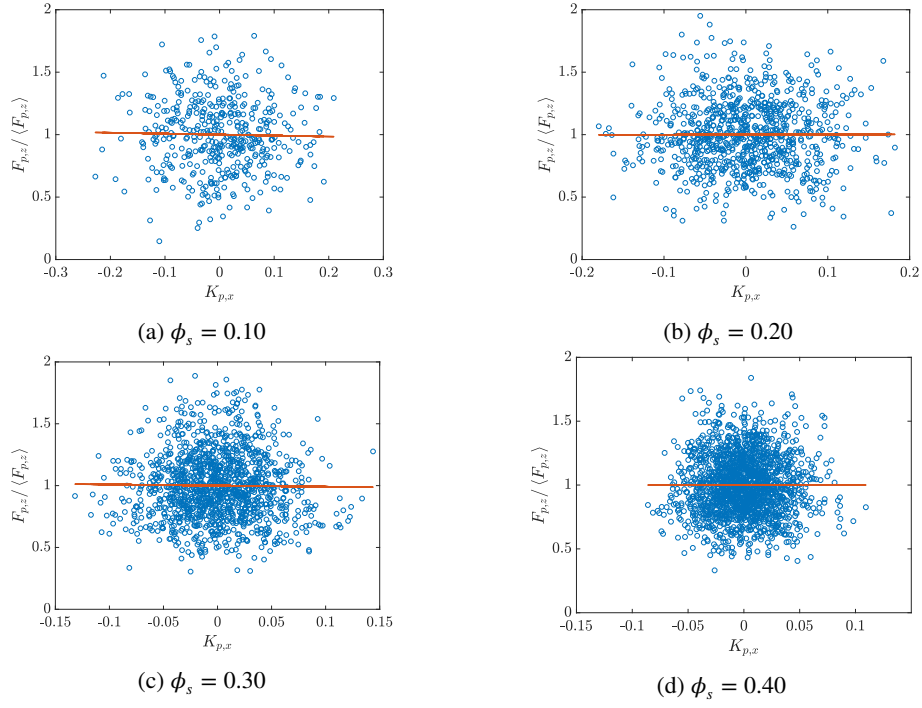


Figure 2.19: Scatter plots and least squares linear regression between $K_{p,x}$ and $F_{p,z}$ for the cases at $Re_p = 50$.

Table 2.5: Square of the Pearson correlation coefficient between $F_{p,z}$ and $K_{p,z}$ and between $F_{p,z}$ and $\beta_{p,z}$.

	$Re_p = 10$				$Re_p = 50$				$Re_p = 100$			
ϕ_s	0.10	0.20	0.30	0.40	0.10	0.20	0.30	0.40	0.10	0.20	0.30	0.40
$\rho_{K_{p,z}, F_{p,z}}^2$	0.07	0.05	0.01	0.01	0.06	0.09	0.04	0.04	0.05	0.09	0.04	0.04
$\rho_{\beta_{p,z}, F_{p,z}}^2$	0.61	0.69	0.65	0.71	0.57	0.62	0.62	0.68	0.51	0.56	0.60	0.63
Σ	0.68	0.74	0.66	0.72	0.63	0.71	0.66	0.72	0.56	0.65	0.64	0.67

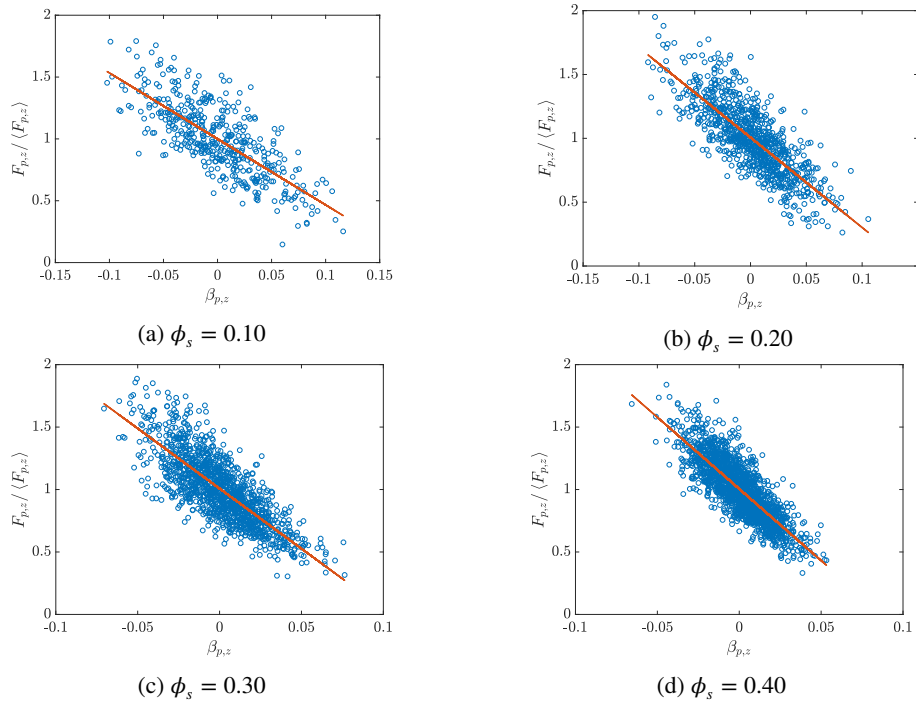


Figure 2.20: Scatter plots and least squares linear regression between $\beta_{p,z}$ and $F_{p,z}$ for the cases at $\text{Re}_p = 50$.

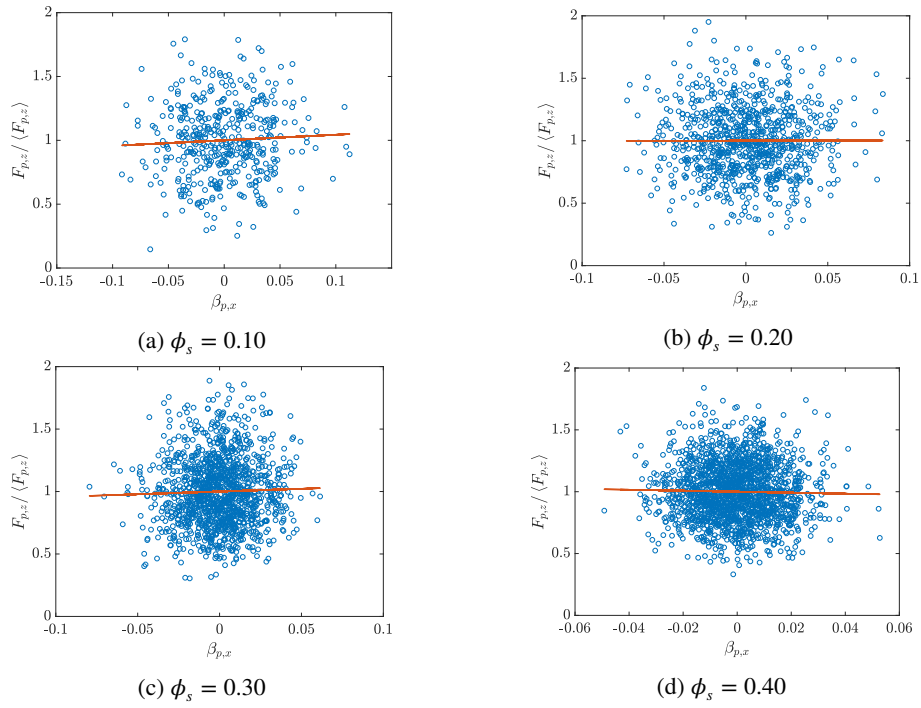


Figure 2.21: Scatter plots and least squares linear regression between $\beta_{p,x}$ and $F_{p,z}$ for the cases at $\text{Re}_p = 50$.

2.5.2 Transverse force component

As detailed in Section 2.3, both the magnitude $F_{p\perp}$ and the direction $\mathbf{e}_\perp$ of the fluid force transverse component must be modeled. A possible way to model $\mathbf{e}_\perp$ is to compare its orientation with that of $\mathbf{e}_\perp^*$ and $\mathbf{e}_\perp^{**}$, the unit vectors giving the direction of the transverse components of $\mathbf{K}_p$ and $\boldsymbol{\beta}_p$, respectively. Figure 2.22a shows that the most probable angle between the transverse components of $\mathbf{F}_p$ and $\mathbf{K}_p$ is π , i.e. when the two vectors are opposite. Interestingly, the same observation is made between $\mathbf{F}_p$ and $\boldsymbol{\beta}_p$ in Figure 2.22b, in an even more pronounced way. This finding is in line with previous observations of Akiki et al. [2] and Moore et al. [89] stating that the presence of lateral neighbors has a tendency to push the particle in the perpendicular direction. It must be stressed that $\mathbf{e}_\perp^*$ and $\mathbf{e}_\perp^{**}$ are uncorrelated since we checked the independence of $\boldsymbol{\beta}_p$ and $\mathbf{K}_p$ previously, so that they both provide information to predict the orientation of the transverse force component. From a modeling perspective, it is however more

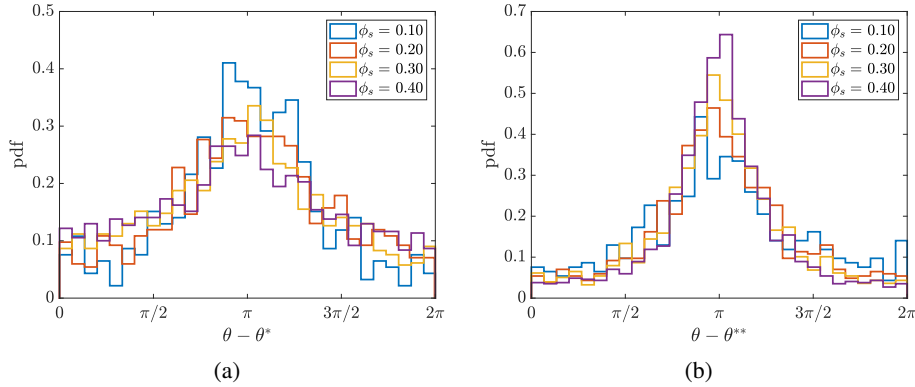


Figure 2.22: Distribution of the phase shift between the transverse components of (a) $\mathbf{F}_p$ and $\mathbf{K}_p$ and (b) $\mathbf{F}_p$ and $\boldsymbol{\beta}_p$.

practical to work with the cartesian components of the transverse force, i.e. $F_{p,x}$ and $F_{p,y}$. For the sake of brevity, we only present the results for $F_{p,x}$. In Figure 2.23, it can be observed that the correlation between $K_{p,x}$ and $F_{p,x}$ yields to a regression line with a negative slope. Negative values of $K_{p,x}$ indicate that the microstructure around the particle is locally oriented towards negative x values. Considering that the x axis is pointing upwards, the resistance to the flow is therefore larger below the particle due to the increased concentration of particles. As a result, the flow is faster above the particle and the upward force exerted on the particle increases. It must be noted that along the streamwise direction the regression line between $K_{p,z}$ and $F_{p,z}$ had a positive

slope (Figure 2.18) because of the shielding effect of the particles located upstream. Regarding the streamwise component of $\mathbf{K}_p$, the scatter plots in Figure 2.24 show that it has no influence on the variability of $F_{p,x}$.

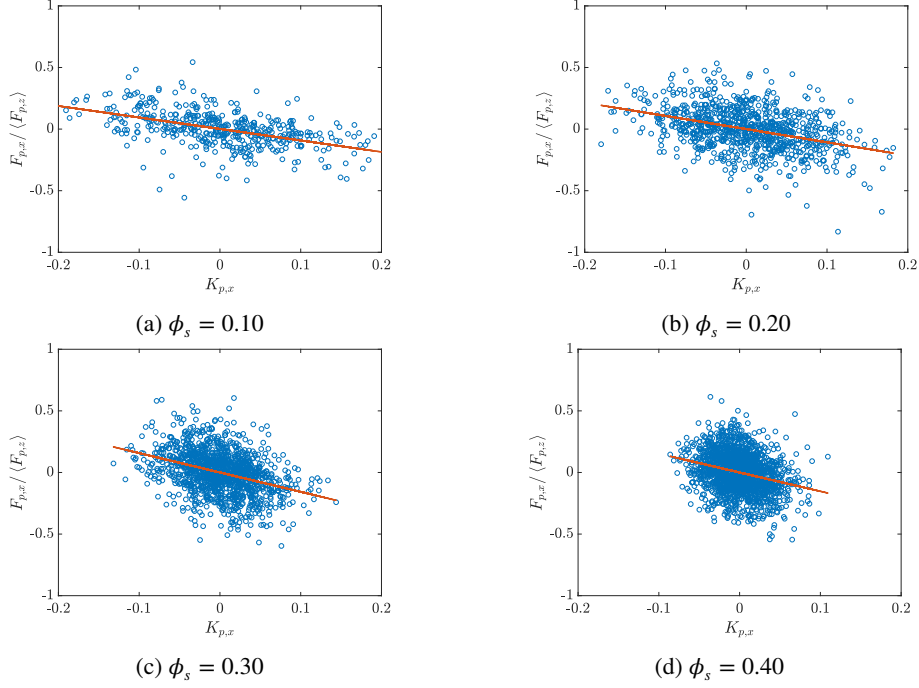


Figure 2.23: Scatter plots and least squares linear regression between $K_{p,x}$ and $F_{p,x}$ for the cases at $\text{Re}_p = 50$.

We now examine the correlation between $F_{p,x}$ and the components of β_p . It appears from Figure 2.25 and Figure 2.26 that $F_{p,x}$ and $\beta_{p,x}$ are fairly correlated, while $F_{p,x}$ and $\beta_{p,z}$ are not. Although not shown here, the same conclusions are drawn between $F_{p,y}$ and $\beta_{p,y}$ and between $F_{p,y}$ and $\beta_{p,z}$, respectively. The square of the correlation coefficient between $F_{p,x}$ and $K_{p,x}$ and between $F_{p,x}$ and $\beta_{p,x}$ is reported in Table 2.6 for the different regimes. The correlation between $F_{p,x}$ and $K_{p,x}$ decreases with ϕ_s while the correlation between $F_{p,x}$ and $\beta_{p,x}$ increases with ϕ_s and decreases with Re_p . Again, dense and viscous regimes yield to more symmetric flow patterns where the predictive capacity of $\beta_{p,x}$ is improved. The Reynolds number sensitivity of the correlation between $F_{p,x}$ and $K_{p,x}$ is less clear as ρ^2 decreases with Re_p in dilute regime while it increases slightly in dense regimes.

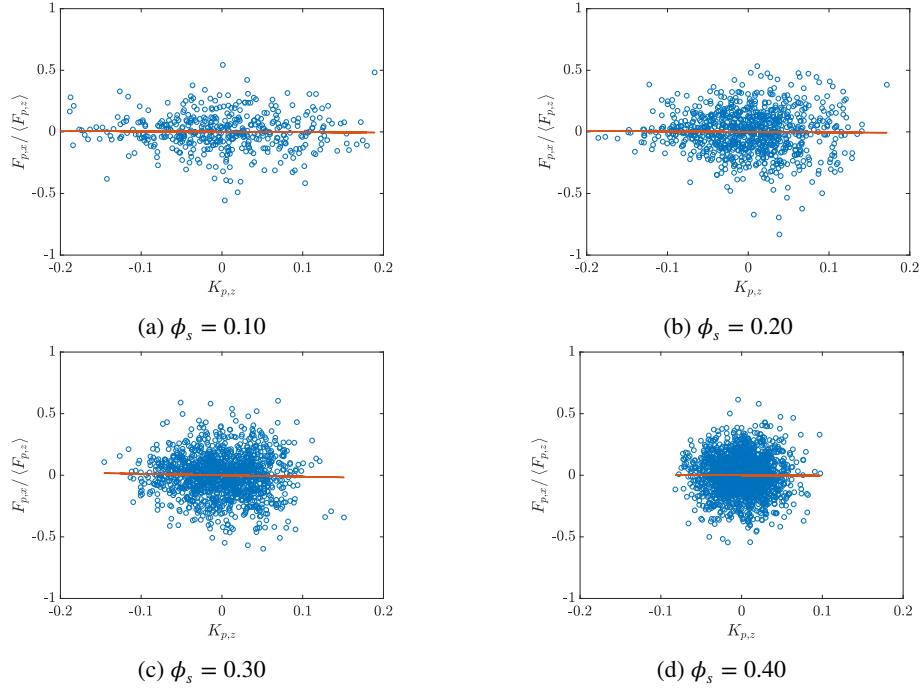


Figure 2.24: Scatter plots and least squares linear regression between $K_{p,z}$ and $F_{p,x}$ for the cases at $Re_p = 50$.

Table 2.6: Square of the Pearson correlation coefficient between $F_{p,x}$ and $K_{p,x}$ and between $F_{p,x}$ and $\beta_{p,x}$.

ϕ_s	$Re_p = 10$				$Re_p = 50$				$Re_p = 100$			
	0.10	0.20	0.30	0.40	0.10	0.20	0.30	0.40	0.10	0.20	0.30	0.40
$\rho_{K_{p,x}, F_{p,x}}^2$	0.26	0.10	0.09	0.04	0.24	0.15	0.13	0.07	0.19	0.13	0.13	0.08
$\rho_{\beta_{p,x}, F_{p,x}}^2$	0.48	0.58	0.62	0.61	0.22	0.35	0.43	0.47	0.16	0.27	0.34	0.38
Σ	0.74	0.68	0.71	0.65	0.46	0.50	0.56	0.54	0.35	0.43	0.47	0.46

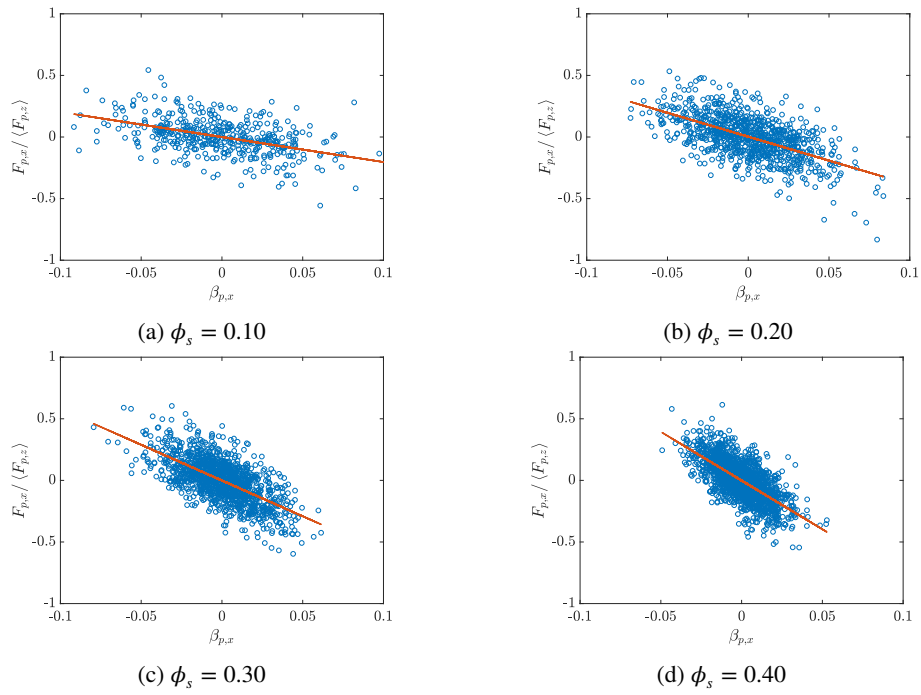


Figure 2.25: Scatter plots and least squares linear regression between $\beta_{p,x}$ and $F_{p,x}$ for the cases at $\text{Re}_p = 50$.

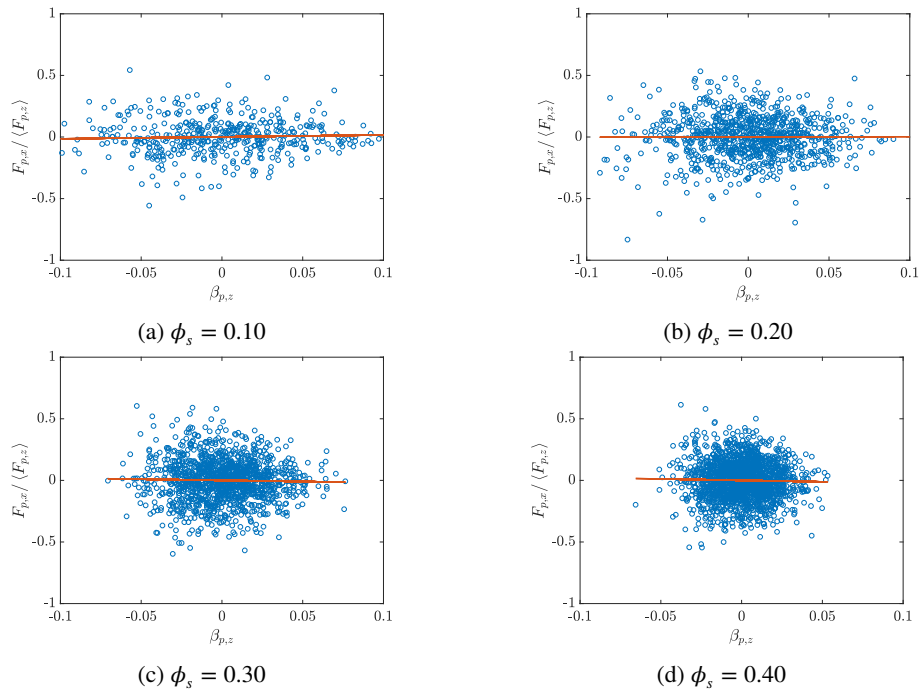


Figure 2.26: Scatter plots and least squares linear regression between $\beta_{p,z}$ and $F_{p,x}$ for the cases at $\text{Re}_p = 50$.

2.6 A multi-linear model for the fluid-particle force

2.6.1 Deterministic model

Based on the above discussions, it appears that the fluid force experienced by a particle immersed in a random array can be partly explained by a few quantities computed from the microstructure formed by the neighboring particles around the reference particle. Isotropic invariants such as $\text{tr}(\mathbf{H}_p)$ turned out to provide little information. On the other hand, the vectors $\mathbf{K}_p$ and $\boldsymbol{\beta}_p$ seem to be able to predict part of the deviation of the fluid force from its mean value. Given the shape of the scatter plots between $\mathbf{F}_p$ and $\boldsymbol{\beta}_p$ in Figures 2.20 and 2.25 and, to a lesser extent, between $\mathbf{F}_p$ and $\mathbf{K}_p$ in Figures 2.18 and 2.23, a deterministic linear model for the force can be formulated as

$$\mathbf{F}_p^{(m)} = \langle F_{p\parallel} \rangle (\mathbf{e}_\parallel + \mathbf{A} \cdot \mathbf{K}_p + \mathbf{B} \cdot \boldsymbol{\beta}_p), \quad (2.37)$$

where $\mathbf{A}$ and $\mathbf{B}$ are two matrices containing the model coefficients and $\langle F_{p\parallel} \rangle$ can be obtained from pre-existing constitutive relations for the mean drag force (see Table 2.1). It must be noted that in the expression of the model given by Eq. (2.37), we removed from Eq. (2.26) the contribution of the random part $\delta\mathbf{F}_p$. The opportunity to add a stochastic contribution to the model is discussed below. Since we showed in previous section that $\mathbf{K}_p$ and $\boldsymbol{\beta}_p$ are independent variables with zero mean, the coefficients of the matrices $\mathbf{A}$ and $\mathbf{B}$ are defined by the following relations:

$$\langle F'_{p,i} K_{p,j} \rangle = \langle F_{p\parallel} \rangle A_{ik} \langle K_{p,k} K_{p,j} \rangle, \quad (2.38)$$

$$\langle F'_{p,i} \beta_{p,j} \rangle = \langle F_{p\parallel} \rangle B_{ik} \langle \beta_{p,k} \beta_{p,j} \rangle. \quad (2.39)$$

Due to the isotropic distribution of the particles in the array, the tensor $\langle K_{p,k} K_{p,j} \rangle$ is also isotropic, so that

$$\langle K_{p,k} K_{p,j} \rangle = \frac{1}{3} \langle K_{p,m} K_{p,m} \rangle \delta_{kj}. \quad (2.40)$$

The counterpart is not true for the tensor $\langle \beta_{p,k} \beta_{p,j} \rangle$. Yet, a general expression for this tensor is given by

$$\langle \beta_{p,k} \beta_{p,j} \rangle = \frac{1}{2} \langle \beta_{p,\perp} \beta_{p,\perp} \rangle \delta_{kj} + \left(\langle \beta_{p,\parallel} \beta_{p,\parallel} \rangle - \frac{1}{2} \langle \beta_{p,\perp} \beta_{p,\perp} \rangle \right) e_{\parallel,k} e_{\parallel,j}. \quad (2.41)$$

In the main reference frame where the direction of the mean flow is aligned with one of the axes, we concluded that $\langle F'_{p,i} K_{p,j} \rangle$ and $\langle F'_{p,i} \beta_{p,j} \rangle$ are diagonal tensors. Hence, taking $\mathbf{e}_\parallel = \mathbf{e}_z$, Eqs. (2.38) to (2.41) simplify drastically and the only non-zero

entries of $\mathbf{A}$ and $\mathbf{B}$ are A_{xx} , A_{yy} , A_{zz} , B_{xx} , B_{yy} and B_{zz} . Then, the expression of $A_{\alpha\alpha}$ and $B_{\alpha\alpha}$ where α is one of the main directions is given by

$$A_{\alpha\alpha} = \frac{\langle F'_{p,\alpha} K_{p,\alpha} \rangle / \langle F_{p\parallel} \rangle}{\langle K_{p,\alpha} K_{p,\alpha} \rangle}, \quad (2.42)$$

$$B_{\alpha\alpha} = \frac{\langle F'_{p,\alpha} \beta_{p,\alpha} \rangle / \langle F_{p\parallel} \rangle}{\langle \beta_{p,\alpha} \beta_{p,\alpha} \rangle}, \quad (2.43)$$

where no summation is performed on α . By symmetry, we also have that $A_{xx} = A_{yy} \triangleq A_{\perp}$ and $B_{xx} = B_{yy} \triangleq B_{\perp}$, which leaves four independent coefficients. Then, Eq. (2.37) reduces to

$$F_{p,x}^{(m)} = \langle F_{p\parallel} \rangle (A_{\perp} K_{p,x} + B_{\perp} \beta_{p,x}), \quad (2.44)$$

$$F_{p,y}^{(m)} = \langle F_{p\parallel} \rangle (A_{\perp} K_{p,y} + B_{\perp} \beta_{p,y}), \quad (2.45)$$

$$F_{p,z}^{(m)} = \langle F_{p\parallel} \rangle (1 + A_{\parallel} K_{p,z} + B_{\parallel} \beta_{p,z}), \quad (2.46)$$

with $A_{\parallel} = A_{zz}$ and $B_{\parallel} = B_{zz}$, in the present case.

The coefficient of determination R^2 of the model given by Eqs. (2.44)-(2.46) for a component α of the force is defined as

$$R^2 = 1 - \frac{\langle (F_{p,\alpha} - F_{p,\alpha}^{(m)})^2 \rangle}{\langle F'^2_{p,\alpha} \rangle}, \quad (2.47)$$

so that $R^2 = 0$ if the model simply returns the mean value of the force and $R^2 = 1$ when the model predicts the exact force on each particle. In the main reference frame, given the expression of the model coefficients (2.42) and (2.43), it can be shown that the theoretical coefficient of determination R^2 reads

$$R^2 = \frac{\langle F'_{p,\alpha} K_{p,\alpha} \rangle^2}{\langle K_{p,\alpha}^2 \rangle \langle F'^2_{p,\alpha} \rangle} + \frac{\langle F'_{p,\alpha} \beta_{p,\alpha} \rangle^2}{\langle \beta_{p,\alpha}^2 \rangle \langle F'^2_{p,\alpha} \rangle} = \rho_{F_{p,\alpha} K_{p,\alpha}}^2 + \rho_{F_{p,\alpha} \beta_{p,\alpha}}^2. \quad (2.48)$$

The expression (2.48) amounts to summing the squares of the Pearson correlation coefficients between $F_{p,\alpha}$ and the corresponding component of $\mathbf{K}_p$ and β_p . Therefore, the last row in Table 2.5 contains the values of the coefficient of determination R^2 associated to the modeling of $F_{p,z}$ from Eq. (2.46) by summing the contributions of $K_{p,z}$ and $\beta_{p,z}$ for the different cases investigated. In the same way, the last row of Table

2.6 contains the values of R^2 associated to the modeling of $F_{p,x}$ from $K_{p,x}$ and $\beta_{p,x}$. Although the contribution of $\mathbf{K}_p$ to the modeling of $F_{p,z}$ is limited with respect to β_p , this is not the case for $F_{p,x}$. Indeed, in some regimes, the contribution of $K_{p,x}$ to the global coefficient of determination exceeds that of $\beta_{p,x}$, which justifies keeping $\mathbf{K}_p$ in the model. The model performs best at low Reynolds number and low volume fraction, with a coefficient of determination $R^2 = 0.74$ for the streamwise component of the force at $(\text{Re}_p, \phi_s) = (10, 0.2)$ and $R^2 = 0.74$ for the transverse component of the force at $(\text{Re}_p, \phi_s) = (10, 0.1)$. The least satisfactory results of the model are found in the prediction of the transverse component of the force at high Reynolds number and low volume fraction, with $R^2 = 0.35$ at $(\text{Re}_p, \phi_s) = (100, 0.1)$. Table 2.7 gives the values of the four independent coefficients obtained from our simulations. The reported $A_\perp$ and $B_\perp$ have actually been computed as the averages between the values obtained for A_{xx} and A_{yy} , and those obtained for B_{xx} and B_{yy} , respectively.

For a potential use in CFD-DEM simulations, a model should be provided for $A_\parallel$, $A_\perp$, $B_\parallel$ and $B_\perp$. The evolution of the model coefficients with Re_p and ϕ_s is depicted in Figure 2.27. First, it can be observed that $B_\parallel$ and $B_\perp$ show a clear linear dependence to ϕ_s . A least-square multi-linear regression yields the following expressions for $B_\parallel$ and $B_\perp$:

$$B_\parallel = -2.6 - 20\phi_s - 0.0068 \text{Re}_p, \quad (2.49)$$

and

$$B_\perp = -0.81 - 20\phi_s + 0.014 \text{Re}_p, \quad (2.50)$$

with values of R^2 associated to the linear regressions equal to 0.978 and 0.993, respectively.

The behavior of $A_\parallel$ and $A_\perp$ is less obvious. The data points for $A_\parallel$ and $A_\perp$ at $\text{Re}_p = 10$ and high volume fraction do not seem to follow the same trend as at higher Reynolds numbers: they correspond to regimes where the contribution of $K_{p,z}$ and (to a lesser extent) $K_{p,x}$ to the variation of the fluid force is weak (see Table 2.5 and 2.6). At $\text{Re}_p = 50$ and $\text{Re}_p = 100$, $A_\parallel$ and $A_\perp$ display almost identical values, which suggests that, beyond a given Re_p , $A_\parallel$ and $A_\perp$ are only sensitive to the volume fraction. Therefore, we propose to distinguish the modeling of $A_\parallel$ and $A_\perp$ between the case at $\text{Re}_p = 10$ on the one hand, and the cases at $\text{Re}_p = 50$ and $\text{Re}_p = 100$ on the other hand:

$$A_\parallel = \begin{cases} 1.1 - 1.2\phi_s, & \text{Re}_p = 10 \\ 0.85 + 1.7\phi_s, & \text{Re}_p = 50, 100 \end{cases} \quad (2.51)$$

and

$$A_\perp = \begin{cases} -0.72 - 1.2\phi_s, & \text{Re}_p = 10 \\ -0.62 - 2.5\phi_s, & \text{Re}_p = 50, 100. \end{cases} \quad (2.52)$$

The larger uncertainty on the fits proposed for $A_{\parallel}$ and $A_{\perp}$ is expected to have a limited impact on the predictive capability of the complete model given the significantly larger values of $B_{\parallel}$ and $B_{\perp}$ in all regimes, while $\mathbf{K}_p$ and β_p are of the same order of magnitude. In any case, additional realizations of the flow should be computed at other values of ϕ_s and Re_p in order to build improved models for $A_{\parallel}$ and $A_{\perp}$.

Table 2.7: Multi-linear model coefficients.

ϕ_s	$Re_p = 10$				$Re_p = 50$				$Re_p = 100$			
	0.10	0.20	0.30	0.40	0.10	0.20	0.30	0.40	0.10	0.20	0.30	0.40
$A_{\parallel}$	0.90	0.95	0.53	0.63	0.93	1.42	1.20	1.42	0.87	1.44	1.35	1.62
$A_{\perp}$	-0.85	-0.89	-1.21	-1.16	-0.86	-1.15	-1.50	-1.50	-0.76	-1.12	-1.52	-1.55
$B_{\parallel}$	-4.98	-6.56	-8.80	-10.26	-5.33	-7.02	-9.60	-11.43	-5.15	-6.75	-9.66	-11.62
$B_{\perp}$	-2.84	-4.62	-6.86	-8.87	-1.94	-3.84	-5.78	-8.11	-1.67	-3.60	-5.31	-7.55

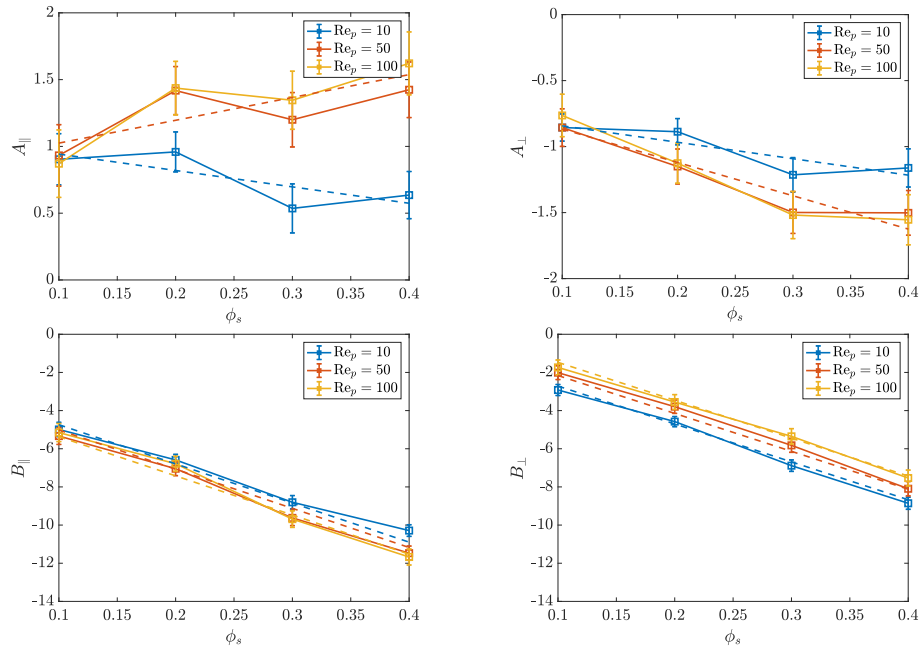


Figure 2.27: Model coefficients as a function of ϕ_s and for different Re_p . The error bars indicate the 95% confidence intervals on the estimates of the model coefficients. The dashed lines correspond to the linear regressions given by Eqs. (2.49), (2.50), (2.51) and (2.52).

To assess the actual performance of the model when the model coefficients $A_{\parallel}$, $A_{\perp}$, $B_{\parallel}$ and $B_{\perp}$ are estimated using the correlations given by Eqs (2.49) to (2.52), a new random array of particles (not used to build the model) has been generated at $\phi_s = 0.30$ and independent realizations of the flow have been computed at $(\text{Re}_p, \phi_s) = (10, 0.30)$, $(\text{Re}_p, \phi_s) = (50, 0.30)$ and $(\text{Re}_p, \phi_s) = (100, 0.30)$. Figure 2.28a shows the regression plots between the three components of the fluid force obtained using the model of Eqs. (2.44)-(2.46) and the values extracted from PR-DNS for the case at $(\text{Re}_p, \phi_s) = (10, 0.30)$. The coefficient of determination for the streamwise component of the force is $R^2 = 0.69$, in good agreement with the theoretical value reported in Table 2.5. Moreover, the model appears to perform equally well along the streamwise and transverse directions in this regime. In Figures 2.28b and 2.28c, the regression plots obtained at higher Reynolds numbers confirm that the performance of the model decreases as we move towards more inertial flows, especially along the transverse directions. Still, the values obtained for R^2 are in lines with those reported in Tables 2.5 and 2.6.

Finally, one realization of the flow was simulated at $(\text{Re}_p, \phi_s) = (70, 0.25)$ to test our microstructure-based model for a set of parameters that were not included in the calibration study. From Figure 2.29, we can conclude that the model performs still very well in predicting the streamwise component of the force with a coefficient of determination $R^2 = 0.71$. In agreement with what has been previously stated, the predictive capability of the model for the transverse components of the force is reduced at higher Reynolds number.

2.6.2 Simple stochastic model

In the expression of the microstructure-based model given by Eq. (2.37), we neglected the random part of the force initially introduced in Eq. (2.26). As a consequence, the variance of the fluid force is not properly reproduced by this model. A stochastic contribution can however be added in order to recover the correct level of force fluctuations. Doing so, Eq (2.37) is modified as

$$\mathbf{F}_p^{(s)} = \langle F_{p\parallel} \rangle (\mathbf{e}_{\parallel} + \mathbf{A} \cdot \mathbf{K}_p + \mathbf{B} \cdot \boldsymbol{\beta}_p + \mathbf{C} \cdot \boldsymbol{\gamma}_p), \quad (2.53)$$

where the superscript (s) indicates the stochastic nature of the model, $\boldsymbol{\gamma}_p$ is a normalized isotropic Gaussian noise uncorrelated to the other model variables $\mathbf{K}_p$ and $\boldsymbol{\beta}_p$, and $\mathbf{C}$ is the standard deviation matrix. By requiring that the model given by Eq. (2.53) recovers the correct variance of the force, it can be shown (see 2.8.2) that $\mathbf{C}$ is diagonal in the

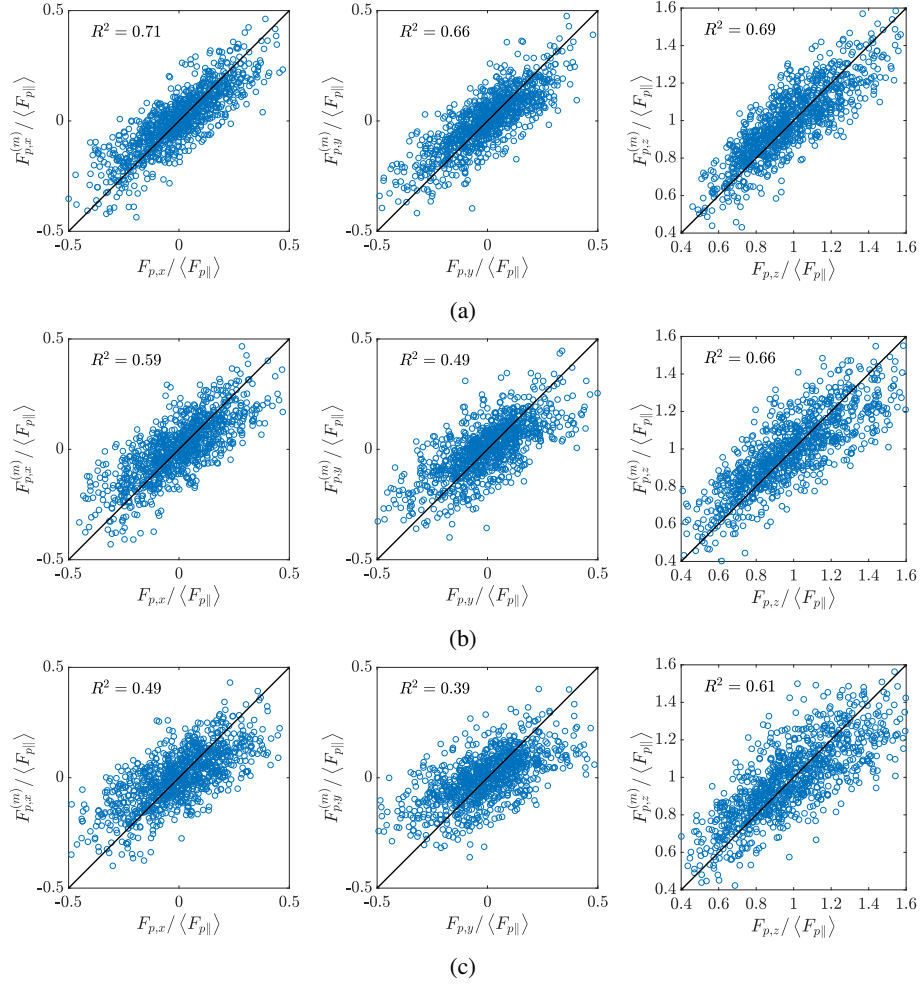


Figure 2.28: Regression plots between the PR-DNS values of the fluid-particle force and the predicted values using the microstructure-based deterministic model given by Eqs (2.44)-(2.46) at $\phi_s = 0.30$ and (a) $\text{Re}_p = 10$, (b) $\text{Re}_p = 50$ and (c) $\text{Re}_p = 100$. Straight lines correspond to the ideal model.

main reference frame, with diagonal values given by

$$C_{\alpha\alpha}^2 = \frac{\langle F_{p,\alpha}^2 \rangle}{\langle F_{p\parallel} \rangle^2} - A_{\alpha\alpha}^2 \langle K_{p,\alpha}^2 \rangle - B_{\alpha\alpha}^2 \langle \beta_{p,\alpha}^2 \rangle, \quad (2.54)$$

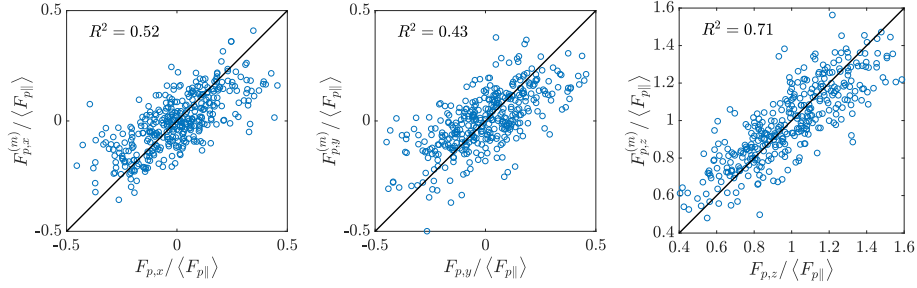


Figure 2.29: Regression plots between the PR-DNS values of the fluid-particle force and the predicted values using the microstructure-based deterministic model given by Eqs (2.44)-(2.46) at $(Re_p, \phi_s) = (70, 0.25)$. Straight lines correspond to the ideal model.

with $\alpha = x, y$ or z , $C_{xx} = C_{yy} = C_{\perp}$ and $C_{zz} = C_{\parallel}$. Then the stochastic model (2.53) reduces to

$$F_{p,x}^{(s)} = \langle F_{p\parallel} \rangle (A_{\perp} K_{p,x} + B_{\perp} \beta_{p,x} + C_{\perp} \gamma_{p,x}) \quad (2.55)$$

$$F_{p,y}^{(s)} = \langle F_{p\parallel} \rangle (A_{\perp} K_{p,y} + B_{\perp} \beta_{p,y} + C_{\perp} \gamma_{p,y}) \quad (2.56)$$

$$F_{p,z}^{(s)} = \langle F_{p\parallel} \rangle (1 + A_{\parallel} K_{p,z} + B_{\parallel} \beta_{p,z} + C_{\parallel} \gamma_{p,z}) \quad (2.57)$$

where $\gamma_{p,x} = \gamma_{p,y} = \gamma_{p,z}$ given the isotropic nature of the Gaussian noise. Values for $C_{\parallel}$ and $C_{\perp}$ are provided in Table 2.8 for the Reynolds numbers and volume fractions we investigated and graphically reported in Figure 2.30.

Table 2.8: Standard deviation coefficients of the Gaussian noise in the stochastic model.

ϕ_s	$Re_p = 10$				$Re_p = 50$				$Re_p = 100$			
	0.10	0.20	0.30	0.40	0.10	0.20	0.30	0.40	0.10	0.20	0.30	0.40
$C_{\parallel}$	0.149	0.125	0.146	0.107	0.179	0.150	0.161	0.125	0.197	0.168	1.172	0.141
$C_{\perp}$	0.077	0.092	0.095	0.090	0.109	0.121	0.116	0.106	0.124	0.139	0.131	0.119

In Figure 2.31, we compare the pdf of the force measured from our PR-DNS results at $(Re_p, \phi_s) = (50, 0.30)$ with the pdf of the force given by the deterministic model (2.37) and by the stochastic model (2.53). As expected, the pdf of the force obtained by the deterministic microstructure-based model is narrower than the pdf of the true force, which means that this model underestimates the variance of the force, i.e. the level of fluctuations. On the other hand, the addition of the random contribution allows to recover the correct shape of the pdf.

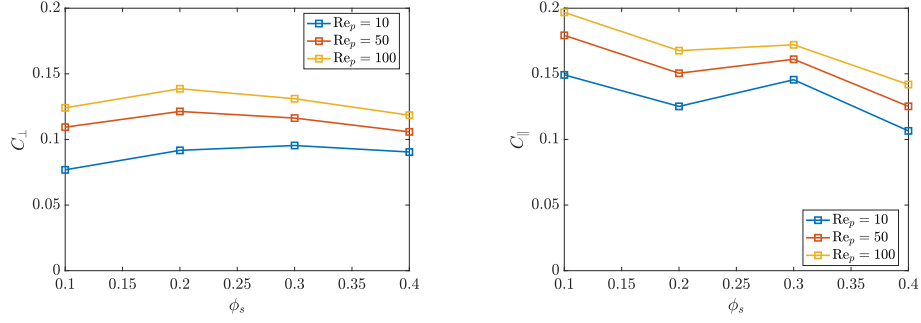


Figure 2.30: Standard deviation coefficients of the stochastic model as a function of the volume fraction and for different Reynolds numbers.

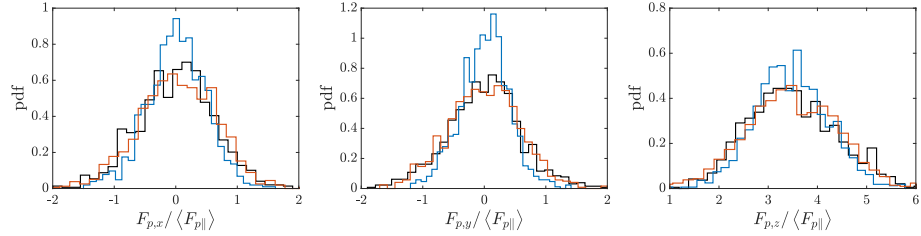


Figure 2.31: Distribution of the cartesian components of the force at $(Re_p, \phi_s) = (50, 0.30)$ obtained from PR-DNS data (—), from the deterministic model (Eqs. (2.44)-(2.46)) (—) and from the stochastic model (Eqs. (2.55)-(2.57)) (—).

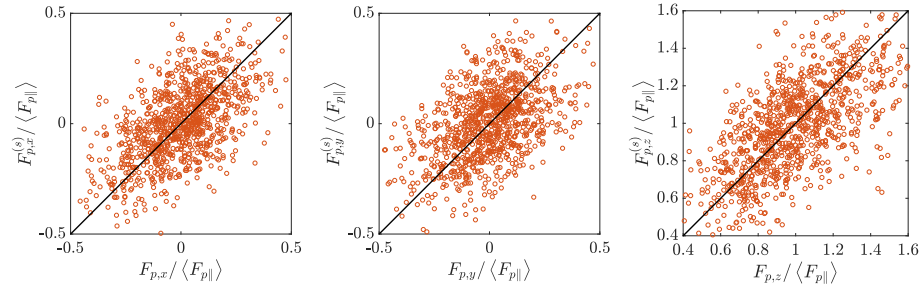


Figure 2.32: Regression plots between the PR-DNS values of the fluid-particle force and the predicted values using the stochastic model given by Eqs. (2.44)-(2.46) at $(Re_p, \phi_s) = (50, 0.30)$. Straight lines correspond to the ideal model.

In Figure 2.32, regression plots compare the PR-DNS values of the force to the values obtained from the stochastic model at $(Re_p, \phi_s) = (50, 0.30)$. It can be observed

that the correlation between the model and the data is less good in comparison to Figure 2.28b. In other words, adding a random fluctuation to our microstructure-based model allows to recover the correct level of force fluctuations, but the price to pay is a reduced correlation between the model and the data. Finally, in a CFD-DEM perspective, the stochastic contribution γ_p should be assigned a time scale related to the lifetime of the microstructure, i.e. how fast the microstructure formed by the surrounding solid particles is modified. Similarly to what was done in [35], resolved simulations with moving particles could be used as a tool to determine the correct time scale to give to the stochastic contribution of the fluid-particle force.

2.7 Conclusions

Current constitutive drag laws used in Euler-Lagrange and Euler-Euler models provide an average value of the force exerted by the fluid on the particles included in the volume of a grid cell. As a result, all particles included in a fluid cell experience the same force, regardless of the local organisation of the solid phase. In this work, we performed particle-resolved simulations of the flow past a fixed array of monodisperse spheres at three Reynolds numbers ($Re_p = 10, 50, 100$) and four volume fractions ($\phi_s = 0.10, 0.20, 0.30, 0.40$) using the direct-forcing immersed boundary detailed in Chapter 1. As previously reported by other groups [2, 110], our results show that the components of the fluid force exerted on a particle immersed in a random array display a significant distribution around their mean values. In this paper, a new physics-based methodology has been introduced in order to capture the distribution of the fluid-particle force. A limited number of quantities inspired from the fabric tensor used in granular media were defined in order to characterize the organization of the microstructure formed by a reference particle and its nearest neighbors. The weight given to a neighbor particle takes the form of a Gaussian filter, so that its contribution decreases with the distance to the reference particle. The statistics of these quantities were studied in detail and their mutual independence was systematically verified. Then, potential correlations between these microstructure characteristic quantities and the fluid-particle force have been investigated. While the trace of $\mathbf{H}_p$ correlates poorly with the force, anisotropic quantities like the components of the vectors $\mathbf{K}_p$ and $\boldsymbol{\beta}_p$ appear to be able to explain part of the fluctuations of the force. Regarding the streamwise component of the force, the main contribution comes from the streamwise component of $\boldsymbol{\beta}_p$. The correlation between $F_{p,z}$ and $\beta_{p,z}$ increases with ϕ_s and decreases with Re_p . The same behavior is observed between the transverse components of the force and those of $\boldsymbol{\beta}_p$. Because it is derived from an even tensor, $\boldsymbol{\beta}_p$ has better predictive capabilities in symmetric flows, i.e. dense and low Reynolds number flows. The contribution of $\mathbf{K}_p$ is less pronounced, but it becomes significant for the transverse components of the force at low volume fraction.

Based on the shape of the scatter plots, we proposed a simple multi-linear deterministic model, using $\boldsymbol{\beta}_p$ and $\mathbf{K}_p$ as independent predictive variables. Since the model is linear with respect to each independent variable, the theoretical coefficient of determination R^2 of the model is readily obtained from the individual Pearson correlation coefficients between the components of the force and those of $\boldsymbol{\beta}_p$ and $\mathbf{K}_p$. The model relies of four independent coefficients $A_{\parallel}$, $A_{\perp}$, $B_{\parallel}$ and $B_{\perp}$ for which simple linear correlations have been proposed as a function of Re_p and ϕ_s in the perspective of a future

use in CFD-DEM. The accuracy of the model was assessed on independent test cases at $Re_p = 10, 50, 100$, using a new random configuration of particles at $\phi_s = 0.3$. It turns out that the theoretical values of R^2 of the model are globally recovered for the three components of the force and for the three Reynolds numbers. This observation shows that the proposed correlations for the coefficients of the model do not significantly deteriorate its predictive capability. As expected, the model performs the best at $Re_p = 10$ as it is able to predict about 70 % of the variability of the three components of the force. In the worst case, the model predicts only 39 % of the variability of the y component of the force for the test case at $Re_p = 100$. Another realization of the flow was computed at $(Re_p, \phi_s) = (70, 0.25)$ to demonstrate the robustness of the model for a set of flow parameters that were not used for building the model. Finally, we showed that the microstructure-based deterministic model underestimates the variance of the fluid-particle force distribution. Therefore, a stochastic model is proposed where the addition of a Gaussian noise allows to recover the correct value of the variance, i.e. the good level of fluctuations of the force. However, we showed that this additional stochastic contribution comes with an increased dispersion and a decreased correlation between the model and the data.

Several improvements to the current methodology are being considered. First, the model has been built with a limited number of tensor quantities. However, the approach introduced in this study is very general and potential correlations between the fluid force and higher moment tensors could be investigated. Furthermore, the expression of the weight function does not currently vary with the Reynolds number (the parameter c is kept constant in Eq. (2.23)), whereas the relative influence of the near neighbors is expected to change with the flow regime. As a corollary, it is aimed to improve the accuracy of the model when the particle Reynolds number increases. The current model should also be tested with moving configurations, e.g. in fluidized beds. In such cases, it has been shown that the mean force experienced by a particle will depend on the density ratio between the two phases (or equivalently the Stokes number) [108, 123]. We should investigate the influence of this factor on the deviation of the fluid-particle force with respect to its mean value. Also, the fluid force experienced by a particle will potentially depends on the velocity distribution of its neighboring particles. An approach similar to that developed in this work could be reproduced using the velocities of the neighboring particles as primitive variables in the definition of the tensor quantities. Finally, the resolved simulation of dynamic particle systems will allow us to extract the lifetime of the microstructure and further use it to provide the correct time scale to the stochastic part of the force model in a CFD-DEM approach. Future work will be dedicated to these various issues.

2.8 Appendices

2.8.1 Independence of microstructure characteristic quantities

Figures 2.33 and 2.34 show the scatter plots between different microstructure characteristic quantities in order to verify their independence.

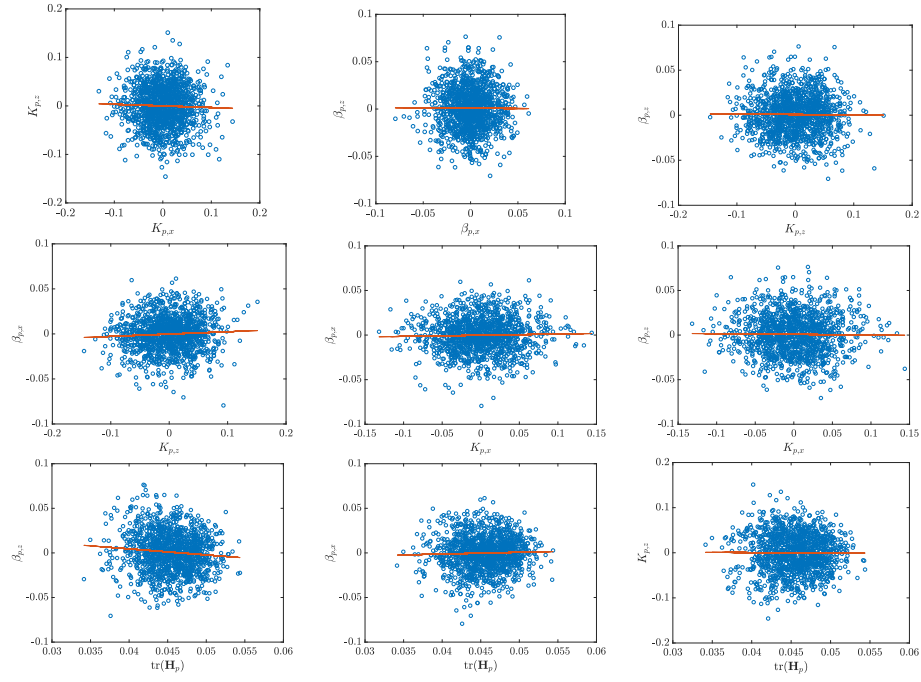


Figure 2.33: Scatter plots and least squares linear regression between different microstructure characteristic quantities for a random arrangement of particles at $\phi_s = 0.30$.

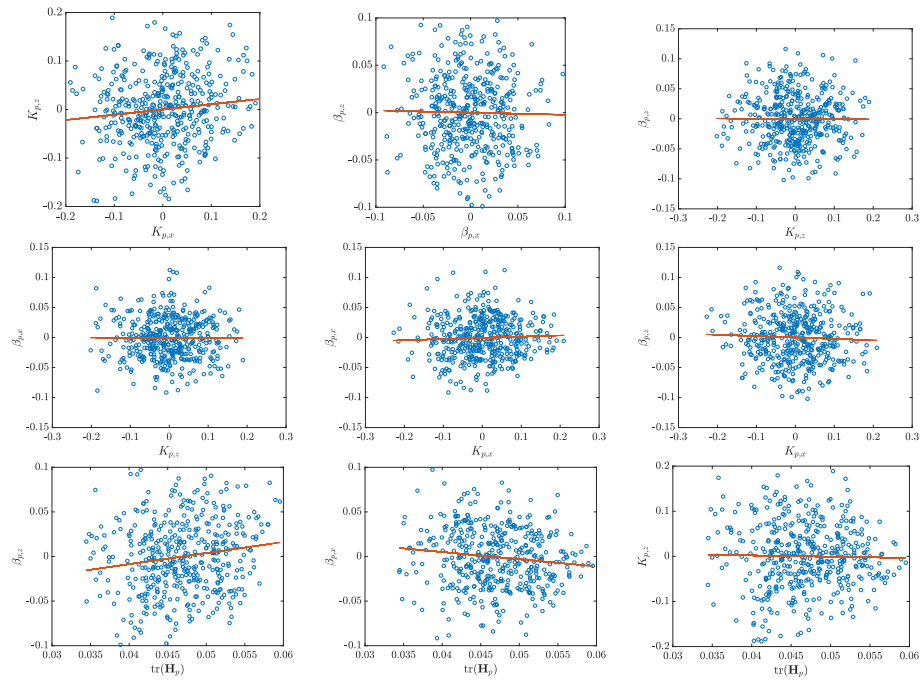


Figure 2.34: Scatter plots and least squares linear regression between different microstructure characteristic quantities for a random arrangement of particles at $\phi_s = 0.10$.

2.8.2 Intensity of the Gaussian noise in the stochastic model

We want to determine the intensity given to the additional Gaussian noise in the stochastic model, i.e. the expression of the matrix $\mathbf{C}$. Using index notation, Eq. (2.53) takes the form

$$F_{p,i}^{(s)} = \langle F_{p\parallel} \rangle (e_{\parallel,i} + A_{ij}K_{p,j} + B_{ij}\beta_{p,j} + C_{ij}\gamma_{p,j}). \quad (2.58)$$

By requiring that the model (2.58) recovers the second-order moments of the force, we can write

$$\begin{aligned} \langle F'_{p,i} F'_{p,j} \rangle &= \langle F_{p,i}^{(s)'} F_{p,j}^{(s)'} \rangle = \langle F_{p\parallel} \rangle^2 (A_{ik}A_{jl} \langle K_{p,k} K_{p,l} \rangle + B_{ik}B_{jl} \langle \beta_{p,k} \beta_{p,l} \rangle \\ &\quad + C_{ik}C_{jl} \langle \gamma_{p,k} \gamma_{p,l} \rangle), \end{aligned} \quad (2.59)$$

where $\langle \gamma_{p,k} \gamma_{p,l} \rangle = \delta_{kl}$ since $\boldsymbol{\gamma}_p$ is a normalized isotropic Gaussian noise. Hence, we have that

$$\langle F'_{p,i} F'_{p,j} \rangle = \langle F_{p\parallel} \rangle^2 (A_{ik}A_{jl} \langle K_{p,k} K_{p,l} \rangle + B_{ik}B_{jl} \langle \beta_{p,k} \beta_{p,l} \rangle + C_{ik}C_{jl}). \quad (2.60)$$

In Figure 2.5, we showed that the individual components of the force are uncorrelated in the main reference frame, i.e. $\langle F'_{p,x} F'_{p,y} \rangle = \langle F'_{p,y} F'_{p,z} \rangle = \langle F'_{p,z} F'_{p,x} \rangle = 0$. It results that the tensor $\langle F'_{p,i} F'_{p,j} \rangle$ is diagonal in the main reference frame. We also showed earlier that A_{ij} and B_{ij} are diagonal in the main reference frame and therefore C_{ij} as well. Hence, the diagonal components of the matrix $\mathbf{C}$ are given by

$$C_{\alpha\alpha}^2 = \frac{\langle F_{p,\alpha}^2 \rangle}{\langle F_{p\parallel} \rangle^2} - A_{\alpha\alpha}^2 \langle K_{p,\alpha}^2 \rangle - B_{\alpha\alpha}^2 \langle \beta_{p,\alpha}^2 \rangle, \quad (2.61)$$

with $\alpha = x, y$ or z .

Heat transfer in the flow past fixed particle arrays

3.1 Introduction

Numerous gas-solid or liquid-solid flows encountered in the industry involve important heat exchanges between the carrying fluid and the solid phase, including biomass pyrolysis, chemical looping combustion or polymerization reactions. The optimal design and control of such equipments requires a detailed understanding of the flow field and heat transfer phenomena at play. Besides experimental characterizations, multi-phase computational fluid dynamics is now commonly used for the design and scale-up of those reactors. Currently, the Euler-Euler (e.g. [91, 109]) and the unresolved Euler-Lagrange models (e.g. [10, 97]) are the two most used methods to simulate pilot-scale or industrial plants. Both approaches rely on closure models to quantify the heat transfer between the solid phase and the gas or the liquid. The modeling strategy is typically based on the calculation of a heat transfer coefficient (or equivalently a Nusselt number) as a function of the flow parameters. In the past decades, many experiments have led to empirical correlations to evaluate the heat transfer coefficient over a wide range of operating conditions [149, 53]. However, those experimental methods rely on the a priori modeling of the temperature profile, typically using simplified 1-D models neglecting axial conduction in the fluid phase. Experimental results are also prone to larger variability depending on measurements techniques and procedures. Particle-resolved simulations (PRS) have recently been used to quantify and model unclosed terms in the large-scale approaches from instantaneous velocity and temperature fields. In particular, many studies have focused on providing accu-

rate Nusselt number correlations that are reliable over a wide range of flow parameters. Early simulations of the heat transfer in flow past fixed arrays of spheres have been performed by Deen et al. [23] and Tavassoli et al. [126] using a ghost-cell and an immersed boundary method, respectively. These authors reported the first Nusselt numbers derived from first principles using resolved simulations. Then, Tavassoli and his co-workers studied fluid-particle heat transfer in fixed arrays of non-spherical particles [127] and in bi-dispersed arrays of spheres [128]. In [134], Tenneti et al. combined their Particle-resolved Uncontaminated-fluid Reconcilable Immersed Boundary Method (PUREIBM) with a thermal self-similarity condition to perform 3-D resolved simulations with heat transfer in fully periodic domains. Wang et al. [151] also extended the semi-analytic Physalis method to handle non-isothermal particle flows. As observed by various authors, Gunn's experimental correlation tends to overestimate the Nusselt number (i.e. the heat transfer efficiency) in particle flows compared to PR-DNS data. Based on numerical simulations, Tenneti et al. [134] and Deen et al. [25] proposed new correlations for the Nusselt number. In [120], Sun et al. developed an improved model for the interfacial heat flux in the Euler-Euler model and, in [121], the same authors proposed a closure for the pseudo-turbulent heat flux (PTHF) term that arises from the correlation between the velocity and temperature fields. Although this term is usually neglected, the authors showed that it can be of the same order of magnitude as the convective mean flux. Recently, Thiam et al. [136] identified a connection between the PTHF and the ratio of two distinct definitions of the Nusselt number and subsequently proposed a model for it.

In this chapter, we first detail the modeling of heat transfer in particle flows at the micro-scale (PR-DNS perspective) and at the macro-scale (Euler-Euler perspective). Then, we use our direct-forcing immersed boundary method to perform several resolved simulations of the flow past statistically homogeneous arrays of spherical particles with heat transfer between the particles and the fluid. These PR-DNS data are further used to compute the interfacial heat flux and the PTHF terms and our results are compared to various closures proposed in the literature. Finally, we focus on the distribution of the fluid-particle heat flux among the particles immersed in the array and we discuss the influence of thermal saturation on reported statistics.

3.2 Heat transfer modeling

3.2.1 Micro-scale flow

Let us consider a two-phase flow system where stationary particles are randomly dispersed in the fluid. At the micro-scale, the fluid phase energy equation in conservative form is given by

$$\frac{\partial}{\partial t} (\rho_f c_{p,f} T) + \nabla \cdot (\rho_f c_{p,f} T \mathbf{u}) = \nabla \cdot (k_f \nabla T). \quad (3.1)$$

By considering that the mean flow is aligned with z direction, the locally scaled temperature is defined as

$$\theta(\mathbf{x}) = \frac{T(\mathbf{x}) - T_s}{T_b(z) - T_s}, \quad (3.2)$$

where T_b is the bulk (or "cup-mixing") temperature. For a fluid with constant density and heat capacity, the bulk temperature is defined as

$$T_b(z) = \frac{\int_{S_f(z)} u_z(\mathbf{x}) T(\mathbf{x}) dS}{\int_{S_f(z)} u_z(\mathbf{x}) dS}, \quad (3.3)$$

where S_f is the surface area occupied by the fluid in a section perpendicular to the mean flow.

When multiple realizations of the micro-scale flows are simulated, the ensemble-averaged bulk temperature is defined as

$$\langle T_b \rangle(z) = \frac{1}{N_\omega} \sum_{\omega=1}^{N_\omega} T_b^{(\omega)}(z), \quad (3.4)$$

where $\langle \cdot \rangle$ is here the ensemble average operator, $T_b^{(\omega)}(z)$ refers to the fluid bulk temperature obtained from a specific realization ω of the flow and N_ω is the total number of realizations.

By considering a control volume V at the micro-scale, it can be shown from a heat balance on Eq. (3.1) (see Appendix C) that, at steady-state, the total heat flux (in [W]) exchanged between the particles and the fluid can be obtained as

$$\mathcal{Q}_{s \rightarrow f} = \int_{\partial V} \chi_f \rho_f c_{p,f} (T \mathbf{u}) \cdot \mathbf{n} dS - \int_{\partial V} \chi_f k_f \nabla T \cdot \mathbf{n} dS. \quad (3.5)$$

where χ_f is the fluid phase indicator function and ∂V corresponds to the boundaries of the control volume. The total heat flux exchanged between the solid and the fluid phases can also be estimated from a Lagrangian perspective as

$$Q_{s \rightarrow f} = - \sum_{i=1}^{N_p^{(V)}} Q_{p,i}, \quad (3.6)$$

where $Q_{p,i}$ is the interfacial heat flux given by Eq. (1.11), i.e. defined positive when heat is transferred *from* the fluid *to* the i th particle and $N_p^{(V)}$ is the number of particles whose center of mass is contained in the control volume V . In the following, the total interfacial heat flux estimated from the fluid phase using Eq. (3.5) will be noted $Q_{s \rightarrow f}^{(f)}$ while we will use the notation $Q_{s \rightarrow f}^{(s)}$ to specify that $Q_{s \rightarrow f}$ has been obtained from the solid phase using individual particle heat fluxes as given by Eq. (3.6). It must be noted that the two quantities may not match exactly since particles will be 'cut' by the boundaries of the control volume and particles are accounted for depending on the location of their center of mass. Obviously, for a control volume containing a sufficient number of particles, $Q_{s \rightarrow f}^{(f)}$ and $Q_{s \rightarrow f}^{(s)}$ should converge to the same value.

3.2.2 Macro-scale flow

The Euler-Euler model equations have been derived by ensemble or volume averaging of the micro-scale flow governing equations [5, 29]. In Appendix C, we detail the averaging procedure of Eq. (3.1) (see also [122, 136]) to obtain the local energy equation of the macro-scale flow,

$$\begin{aligned} \frac{\partial}{\partial t} (\rho_f c_{p,f} \phi_f \langle T^{(f)} \rangle) + \nabla \cdot (\rho_f c_{p,f} \phi_f \langle T^{(f)} \rangle \langle \mathbf{u}^{(f)} \rangle) \\ = \nabla \cdot (k_f \phi_f \nabla \langle T^{(f)} \rangle) + q_{s \rightarrow f} - \nabla \cdot (\rho_f c_{p,f} \phi_f \langle T' \mathbf{u}' \rangle^{(f)}), \end{aligned} \quad (3.7)$$

where $q_{s \rightarrow f}$ is the interfacial heat flux between the solid and the fluid phases per unit volume. In Eq. (3.7), we introduced the fluid-phase ensemble averages of the velocity and temperature fields $\langle \mathbf{u}^{(f)} \rangle$ and $\langle T^{(f)} \rangle$. For an Eulerian quantity ψ , its fluid-phase ensemble average is defined as

$$\langle \psi^{(f)} \rangle (\mathbf{x}) \triangleq \frac{\langle \chi_f(\mathbf{x}) \psi(\mathbf{x}) \rangle}{\phi_f(\mathbf{x})}, \quad (3.8)$$

where χ_f is the fluid phase indicator function and $\phi_f = \langle \chi_f \rangle = 1 - \phi_s$ is the void fraction. For statistically homogeneous quantities, $\langle \psi^{(f)} \rangle$ can be evaluated by spatial

averaging over a statistically representative volume V ,

$$\langle \psi^{(f)} \rangle = \frac{1}{V_f} \int_{V_f} \psi(\mathbf{x}) \, dV = \frac{\int_V \chi_f(\mathbf{x}) \psi(\mathbf{x}) \, dV}{\int_V \chi_f(\mathbf{x}) \, dV}, \quad (3.9)$$

where V_f is the volume occupied by the fluid phase inside the volume V . Conveniently, PR-DNS can be used to obtain estimates of ensemble averages based on a limited number of flow configurations given the equivalency between spatial and ensemble averages for statistically homogeneous quantities. In the following, some quantities will be statistically inhomogeneous along the streamwise direction. In that case, we can define the fluid-phase cross-sectional average of ψ at a streamwise position z as

$$\langle \psi^{(f)} \rangle(z) = \frac{1}{S_f(z)} \int_{S_f(z)} \psi(\mathbf{x}) \, dS = \frac{\int_{S(z)} \chi_f(\mathbf{x}) \psi(\mathbf{x}) \, dS}{\int_{S(z)} \chi_f(\mathbf{x}) \, dS}. \quad (3.10)$$

where S is the cross section of the volume V . In practice, the bulk temperature at a streamwise location z is similarly evaluated as

$$T_b(z) = \frac{\int_S \chi_f(\mathbf{x}) u_z(\mathbf{x}) T(\mathbf{x}) \, dS}{\int_S \chi_f(\mathbf{x}) u_z(\mathbf{x}) \, dS}. \quad (3.11)$$

The fluctuation of ψ with respect to its phase average is defined as

$$\psi'(\mathbf{x}) = \psi(\mathbf{x}) - \langle \psi^{(f)} \rangle(\mathbf{x}). \quad (3.12)$$

and $\langle \psi'^{(f)} \rangle = 0$ by definition. The last term of Eq. (3.7) corresponds to the energy transport induced by the correlation between the temperature and the velocity fields at the micro-scale and is usually referred to as a pseudo-turbulent heat flux (PTHF) [121, 136]. Although this term is usually neglected, Sun et al. [121] showed that it can represent 40% to 100% of the convective mean flux. These authors also report that the contribution of the PTHF increases with the the solid volume fraction due to larger fluctuations in the flow fields. Therefore, both the interfacial and the pseudo-turbulent heat fluxes require closures. In the following, we detail how PR-DNS can be used to model these unclosed terms.

Finally, for statistically inhomogeneous quantities, the streamwise average of $\langle \psi^{(f)} \rangle$ is defined by

$$\langle \psi^{(f)} \rangle_m = \frac{1}{L} \int_0^L \langle \psi^{(f)} \rangle(z) dz \quad (3.13)$$

where L is the length of the control volume.

3.3 Simulation of the flow with heat transfer past a fixed array of spheres

3.3.1 Numerical set-up

We consider the heat transfer in the flow past a random array of monodisperse spherical particles as shown in Figure 3.1. At the inflow, the fluid has a prescribed velocity

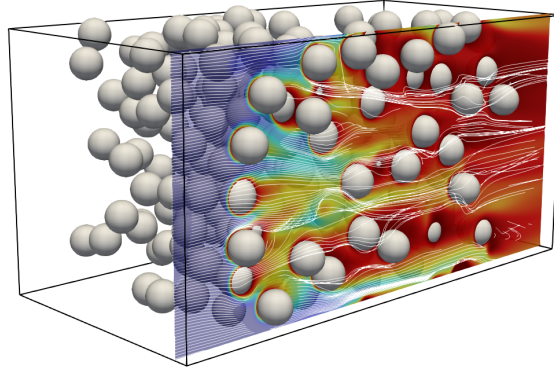


Figure 3.1: Heating of a fluid as it flows past a random array of hot spheres with constant temperature at $(Re_p, Pr, \phi_s) = (50, 1, 0.20)$. Iso-contours of the temperature field in a plane aligned with the streamwise direction and streamlines of the flow.

$\mathbf{U}_0 = U_0 \mathbf{e}_z$ and temperature T_0 . Natural outflow conditions are imposed at the outlet and periodic boundary conditions are used in the transverse directions. The solid particles have a fixed temperature T_s prescribed using our immersed Boundary Method presented in Chapter 1. The computational domain has dimensions $L_x = L_y = 8d_p$ and $L_z = 16d_p$. The inflow is located at $z = -2d_p$ and particles are randomly distributed between $z = 0$ and $z = L_{\text{bed}} = 12d_p$. Resolved simulations have been performed at

$Re_p = \frac{U_0 d_p}{\nu} = (10, 50, 100)$ and solid volume fractions $\phi_s = (0.10, 0.20, 0.30, 0.40)$. The Prandtl number is unity. The grid resolution increases with the Reynolds number: $N_d = \frac{d_p}{h} = 16$ at $Re_p = 10$, $N_d = 24$ at $Re_p = 50$ and $N_d = 32$ at $Re_p = 100$. The number of particles is determined as

$$N_p = \frac{\phi_s V_{bed}}{V_p} = \frac{6\phi_s V_{bed}}{\pi d_p^3}, \quad (3.14)$$

with $V_{bed} = L_x L_y L_{bed}$. Hence, the array contains 147 particles at $\phi_s = 0.1$, 294 at $\phi_s = 0.2$, 440 at $\phi_s = 0.3$ and 587 at $\phi_s = 0.4$. To reduce the statistical variability induced by a specific arrangement of particles, multiple independent realizations of the flow corresponding to different random particle configurations are simulated. In the following, statistics are averaged over 5 independent realizations for each pair (Re_p, ϕ_s) . For the regimes we investigated, the flow is steady after an initial transient. The reported results are those obtained at steady-state.

3.3.2 Inhomogeneity of the thermal problem

In Figures 3.2a and 3.2b, we plot the streamwise profiles of the bulk temperature $\langle T_b \rangle$ and the fluid-phase averaged temperature $\langle T^{(f)} \rangle$ at $Re_p = 50$ and for $\phi_s = 0.1, 0.2, 0.3, 0.4$. Since the flow is heated up by the particles, the thermal problem is statistically inhomogeneous in the streamwise direction and the driving force for the heat transfer (i.e. the temperature difference between the two phases) decreases. It can be observed that thermal saturation happens sooner when the solid volume fraction increases. Indeed, the specific area a_p (i.e. the solid phase surface area per unit volume in $[1/m]$) is given by $a_p = \frac{6\phi_s}{d_p}$, meaning that the surface area available for heat transfer increases linearly with the solid volume fraction of the array.

As noted by Sun et al. [121], the heat transfer problem in the flow past a fixed array of particles is analogous, in an average sense, to the heat transfer in a pipe flow. Hence, the heat balance for the bulk temperature $\langle T_b \rangle$ when axial conduction is neglected reads

$$\frac{d \langle T_b \rangle}{dz} = \frac{a_p h_b}{\rho_f c_{p,f} U_0} (T_s - \langle T_b \rangle). \quad (3.15)$$

where h_b is the heat transfer coefficient (in $[W/(m^2 K)]$) based on the bulk temperature. The solution to Eq. (3.15) is given by

$$\log \left(\frac{\langle T_b \rangle(z) - T_s}{T_0 - T_s} \right) = - \frac{a_p h_b}{\rho_f c_{p,f} U_0} z, \quad (3.16)$$

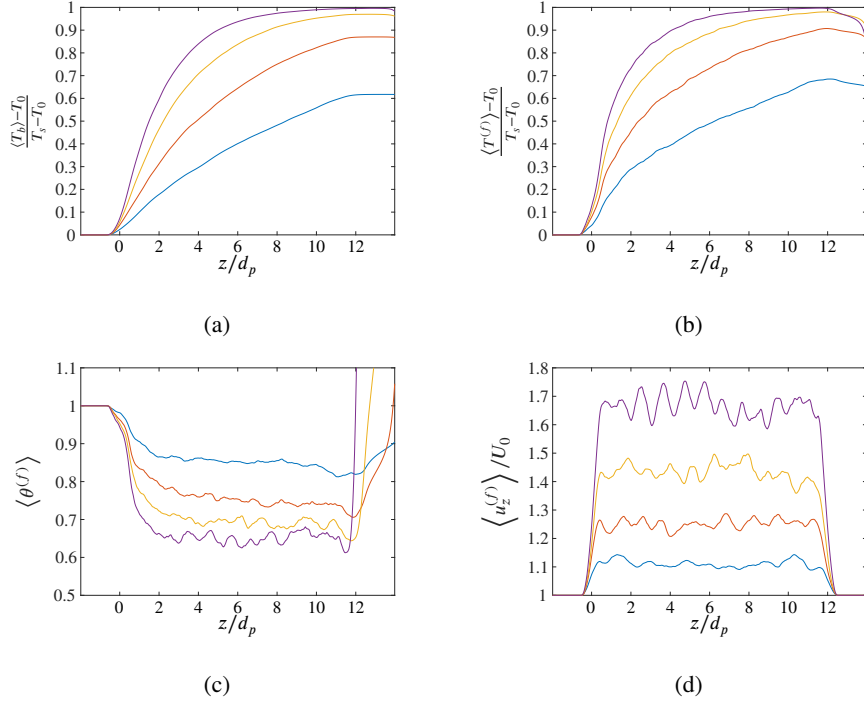


Figure 3.2: Streamwise profile of (a) the bulk temperature $\langle T_b \rangle$, (b) the fluid-phase averaged temperature $\langle T^{(f)} \rangle$, (c) the fluid-phase averaged scaled temperature $\langle \theta^{(f)} \rangle$ and (d) the fluid-phase averaged streamwise velocity component $\langle u_z^{(f)} \rangle$ at $(\text{Re}_p, \text{Pr}) = (50, 1)$ and for the volume fractions $\phi_s = 0.1$ (—), $\phi_s = 0.2$ (—), $\phi_s = 0.3$ (—) and $\phi_s = 0.4$ (—).

From Eq. (3.15), we can identify the heat transfer characteristic length scale,

$$L_h = \frac{\rho_f c_{p,f} U_0}{a_p h_b} = \frac{\text{Pe } d_p}{6\phi_s \text{Nu}_b}, \quad (3.17)$$

where $\text{Nu}_b = \frac{h_b d_p}{k_f}$ is the Nusselt number and $\text{Pe} = \text{Pr } \text{Re}_p$ is the Péclet number. The solution to Eq. (3.15) can be recast as

$$\frac{\langle T_b \rangle(z) - T_0}{T_s - T_0} = 1 - \exp\left(-\frac{z}{L_h}\right), \quad (3.18)$$

which means that, at $z = L_h$, the fluid has covered $\left(1 - \frac{1}{e}\right) = 63\%$ of its potential temperature rise. From the definition of L_h , it results that the fluid reaches thermal sat-

uration faster as Pe decreases and ϕ_s increases. For the set of parameters $(Re_p, Pr, \phi_s) = (50, 1, 0.4)$ and with $Nu_b \simeq 9$ in this regime (see Figure 3.6b later), Eq. (3.17) yields

$$\frac{L_h}{d_p} \simeq 2.3 \quad (3.19)$$

Hence, in this regime, most of the heat transfer is performed by the first three rows of particles, as observed in Figure 3.2a. The impact of the solid volume fraction on the thermal saturation can also be visualized in Figure 3.3 where we show iso-contours of the temperature field at $Re_p = 50$ and for increasing values of ϕ_s . At high volume fraction, it can be seen that only the first part of the bed actually participates in heat transfer as the temperature of the fluid rapidly reaches that of the solid.

By analogy with pipe flows, the flow in a fluid-particle system is considered thermally fully developed when [134]

$$\frac{\partial \langle \theta^{(f)} \rangle}{\partial z} = 0. \quad (3.20)$$

In the present work, a thermal entrance zone exists at the beginning of the particle array because of the inflow condition prescribed at the inlet of the domain. Figure 3.2c confirms that

$$\langle \theta^{(f)} \rangle(z) = \frac{\langle T^{(f)} \rangle(z) - T_s}{\langle T_b \rangle(z) - T_s} \quad (3.21)$$

is fairly constant along the streamwise direction after the entrance and before the exit buffer zone of the domain. To report good statistics, quantities of interest will be measured in a region bounded by the streamwise positions $z_a = 2d_p$ and $z_b = 10d_p$ where the flow can be considered to be thermally fully developed. The boundaries of this control volume are indicated by the black boxes superimposed to the temperature iso-contours in Figure 3.3. Finally, Figure 3.2d shows that the streamwise velocity component is also statistically homogeneous, which confirms the homogeneous distribution of the particles in the array given that $\langle u_z^{(f)} \rangle = U_0/(1 - \phi_s)$.

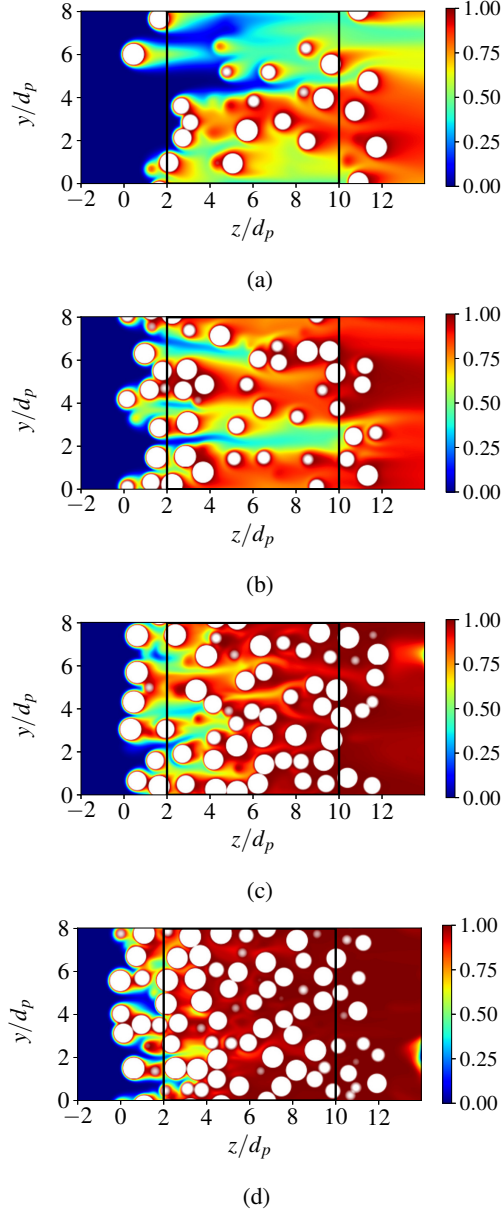


Figure 3.3: Heat transfer in the flow past a random array of spheres: iso-contours of the normalized temperature field $\frac{T-T_0}{T_s-T_0}$ in a yz plane at $(\text{Re}_p, \text{Pr}) = (50, 1)$ and (a) $\phi_s = 0.10$, (b) $\phi_s = 0.20$, (c) $\phi_s = 0.30$ and (d) $\phi_s = 0.40$.

3.3.3 Interfacial heat flux and Nusselt number evaluation

The interfacial heat flux in the Euler-Euler energy equation (Eq. (3.7)) is classically modelled as

$$q_{s \rightarrow f} = h_f a_p (T_s - \langle T^{(f)} \rangle), \quad (3.22)$$

where h_f is the heat transfer coefficient based on the fluid-phase averaged temperature. In the Euler-Euler approach, the heat transfer coefficient is obtained from the Nusselt number Nu_f as

$$h_f = \frac{\text{Nu}_f k_f}{d_p}, \quad (3.23)$$

and the interfacial heat transfer term is closed given that the Nusselt number is provided. From a PR-DNS perspective, conversely, the Nusselt number based on the fluid-phase averaged temperature can be obtained as

$$\text{Nu}_f = \frac{q_{s \rightarrow f}^{(\text{DNS})} d_p^2}{6\phi_s (T_s - \langle T^{(f)} \rangle_m) k_f}, \quad (3.24)$$

where

$$q_{s \rightarrow f}^{(\text{DNS})} = \frac{Q_{s \rightarrow f}}{V}, \quad (3.25)$$

and

$$\langle T^{(f)} \rangle_m = \frac{1}{(z_b - z_a)} \int_{z_a}^{z_b} \langle T^{(f)} \rangle(z) dz \quad (3.26)$$

are statistical estimates obtained from resolved simulations for $q_{s \rightarrow f}$ and $\langle T^{(f)} \rangle$, respectively.

From a PR-DNS perspective, it is also possible to define a *local* interfacial heat flux. Since the flow is aligned with the z direction and periodic boundary conditions are used for the transverse directions, Eq. (3.5) takes the simpler form

$$Q_{s \rightarrow f} = \left(\int_{S_b} \chi_f \rho_f c_{p,f} T u_z dS - \int_{S_b} \chi_f k_f \frac{\partial T}{\partial z} dS \right) - \left(\int_{S_a} \chi_f \rho_f c_{p,f} T u_z dS - \int_{S_a} \chi_f k_f \frac{\partial T}{\partial z} dS \right), \quad (3.27)$$

where S_a and S_b correspond to the surfaces at the inlet and outlet of the control volume bounded by the streamwise positions z_a and z_b . From Eq. (3.27), we define the conductive and convective heat fluxes at a given streamwise location z as

$$Q_{\text{conv}}(z) \triangleq \int_{S(z)} \chi_f \rho_f c_{p,f} u_z T dS, \quad (3.28)$$

and

$$Q_{\text{cond}}(z) \triangleq - \int_{S(z)} \chi_f k_f \frac{\partial T}{\partial z} dS \quad (3.29)$$

respectively. The local volumetric interfacial heat flux (in $[\text{W}/\text{m}^3]$) at a streamwise location z can thus be defined as

$$q_v(z) = \frac{1}{S} \frac{d}{dz} (Q_{\text{conv}}(z) + Q_{\text{cond}}(z)). \quad (3.30)$$

Then, the average heat flux exchanged between the solid and the fluid phases per unit volume reads

$$q_{s \rightarrow f}^{(\text{DNS})} = q_{v,m} = \frac{1}{L} \int_{z_a}^{z_b} q_v(z) dz. \quad (3.31)$$

From Eq. (3.30), we can define a local Nusselt number based on the bulk temperature at a given streamwise position as

$$\text{Nu}_b(z) = \frac{q_v(z) d_p}{a_p k_f (T_s - \langle T_b \rangle(z))}. \quad (3.32)$$

Tenneti et al. [134] showed that, although the bulk temperature and the volumetric heat flux (respectively given by Eqs (3.3) and Eq. (3.30)) vary along the streamwise direction, the Nusselt number defined by Eq. (3.32) is constant along the streamwise direction when the flow is developed. This finding is also evidenced in Figure 3.4 where we show the streamwise profile of the local Nusselt number defined by Eq. (3.32) for the case $(\text{Re}_p, \phi_s) = (50, 0.2)$. After the entrance region and before the buffer zone at the outlet, it can be observed that the Nusselt number is essentially constant. As a result, taking the streamwise average of Eq. (3.32) gives us an expression to estimate the (homogeneous) Nusselt number from our DNS results:

$$\text{Nu}_b = \text{Nu}_{b,m} = \frac{q_{s \rightarrow f}^{(\text{DNS})} d_p^2}{6 \phi_s k_f (T_s - \langle T_b \rangle_m)}. \quad (3.33)$$

In Figure 3.4, we show that the mean Nusselt number calculated as the streamwise average of Eq. (3.32) and as given by Eq. (3.33) yield virtually the same value, as expected.

Similarly to what is done in experimental studies, the Nusselt number can be simply estimated from the bulk temperature profile. Using the 1-D model given by Eq. (3.15), the bulk temperature is fitted in logarithmic scale to a linear model in the thermally developed region, as shown in Figure 3.5. Doing so, the heat transfer coefficient h_b can be straightforwardly extracted from the slope of the linear regression (see Eq. (3.16)).

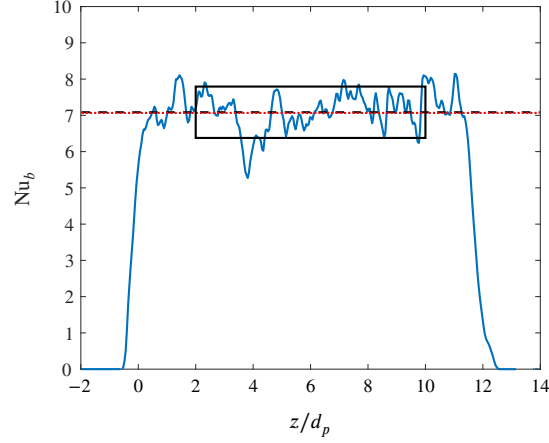


Figure 3.4: Local Nusselt number (Eq. (3.32)) as a function of the streamwise position along the bed (—) at $(\text{Re}_p, \text{Pr}, \phi_s) = (50, 1, 0.2)$. Comparison between the streamwise average of Eq. (3.32) in the box bounded by $z_a = 2d_p$ and $z_b = 10d_p$ (--) and the average Nusselt number given by Eq. (3.33) (····).

Several correlations have been proposed in the literature to compute the Nusselt number in particle flows, without systematically specifying whether they refer to Nu_b (based on the bulk temperature) or Nu_f (based on the fluid-phase averaged temperature). Gunn [53] first proposed an empirical correlation derived from experimental data to relate the Nusselt number to the particle Reynolds number, Prandtl number and bed void fraction:

$$\text{Nu} = \left(7 - 10\phi_f + 5\phi_f^2\right) \left(1 + 0.7 \text{Re}_p^{0.2} \text{Pr}^{1/3}\right) + \left(1.33 - 2.4\phi_f + 1.2\phi_f^2\right) \text{Re}_p^{0.7} \text{Pr}^{1/3}, \quad (3.34)$$

$$0.35 \leq \phi_f \leq 1.0, \quad 1 \leq \text{Re}_p \leq 10^5.$$

It was however reported by several studies [126, 134, 120, 136] that Gunn's correlation has a tendency to overestimate the heat transfer between the two phases when T_b is taken as the reference temperature. Correlations for Nu_b based on PR-DNS results were separately proposed by Deen et al. [25] and Sun et al. [120]:

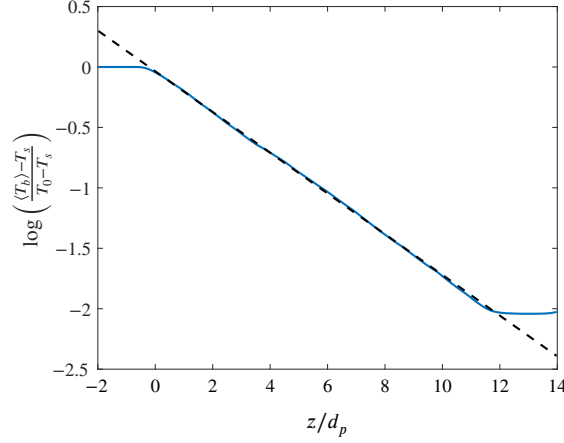


Figure 3.5: Logarithmic profile of the bulk temperature obtained from PR-DNS at $(Re_p, Pr, \phi_s) = (50, 1, 0.20)$ (—) and corresponding linear fit (--) between $z_a = 2d_p$ and $z_b = 10d_p$.

Deen et al. [25]

$$Nu = \left(7 - 10\phi_f + 5\phi_f^2\right) \left(1 + 0.17 Re_p^{0.2} Pr^{1/3}\right) + \left(1.33 - 2.31\phi_f + 1.16\phi_f^2\right) Re_p^{0.7} Pr^{1/3}, \quad (3.35)$$

$$0.50 \leq \phi_f \leq 1.0, \quad 10 \leq Re_p \leq 100,$$

Sun et al. [120]

$$Nu = \left(-0.46 + 1.77\phi_f + 0.69\phi_f^2\right) / \phi_f^3 + \left(1.37 - 2.4\phi_f + 1.2\phi_f^2\right) Re_p^{0.7} Pr^{1/3}, \quad (3.36)$$

$$0.50 \leq \phi_f \leq 1.0, \quad 1 \leq Re_p \leq 100.$$

We report in Figure 3.6 the values for Nu_b obtained from our PR-DNS data at the three Reynolds numbers and the four volume fractions investigated. The Nusselt number has been estimated in three ways: (1) using $Q_{s \rightarrow f}^{(f)}$, the interfacial heat flux obtained from the fluid phase heat balance (Eq. (3.5)), (2) using $Q_{s \rightarrow f}^{(s)}$ the interfacial heat flux obtained from individual particle heat fluxes (Eq. (3.6)) and (3) using the log-linear regression on the bulk temperature profile (Eq. (3.16)). It appears that the heat flux (and thus the Nusselt number) calculated from the solid phase is always larger

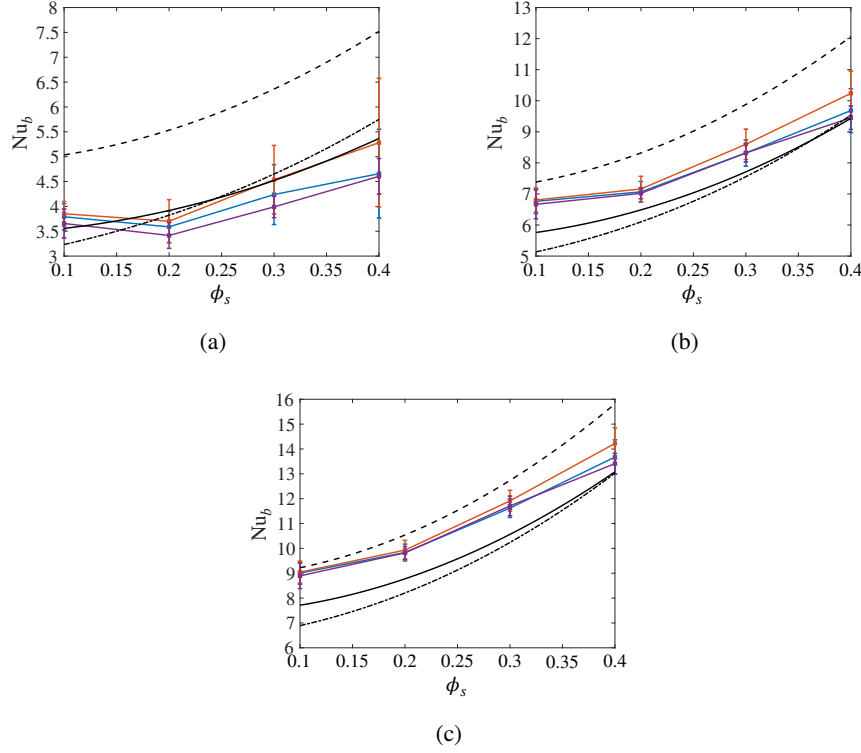


Figure 3.6: Evolution of Nu_b with the solid volume fraction at $Pr = 1$ and (a) $Re_p = 10$, (b) $Re_p = 50$ and (c) $Re_p = 100$. The Nusselt number is evaluated from a fluid phase heat balance ($\square$), individual particle heat fluxes ($\square$) and a log-linear regression on the bulk temperature profile ($\square$). Error bars indicate 95% confidence interval on the mean value. Comparison with Deen et al. [25] (—), Sun et al. [120] (---) and Gunn's [53] (- -) correlations.

than that computed from the fluid phase heat balance. The deviation is the largest at $(Re_p, \phi_s) = (10, 0.4)$ with $Q_{s \rightarrow f}^{(s)}$ being 13.8% higher than $Q_{s \rightarrow f}^{(f)}$. As a general trend, the uncertainty of the results increases for the regimes where the thermal saturation occurs very fast, i.e. at high ϕ_s and low Re_p . Indeed, in those regimes, the estimation of the mean interfacial heat flux per unit volume $q_{s \rightarrow f}^{(DNS)}$ and the temperature difference $(T_s - \langle T_b \rangle_m)$ will approach zero in the control volume, so that the evaluation of Nu_b from Eq. (3.33) will be subject to more variations between two realizations of the flow. The agreement between our PR-DNS results and previous literature correlations is globally

satisfactory, although at high Reynolds number and low solid volume fraction, the Nusselt number appears to be significantly higher than that provided by the correlations of Sun et al. [120] and Deen et al. [25]. This can potentially be explained by the thermal entrance effect and the improved heat transfer in the first particle rows of the bed. We attempted to use a smaller control volume with the left boundary z_a located further downstream (we tested $z_a = 4d_p$ and $z_a = 6d_p$) to further limit the thermal entrance effect. Yet, we did not notice any significant change in the value of Nu_b . We also observe that at $(Re_p, \phi_s) = (10, 0.4)$ (i.e. fast thermal saturation), the Nusselt number evaluated from a fluid-phase heat balance is significantly lower than the values predicted by the correlations of Sun et al. [120] or Deen et al. [25]. We also tried to increase the grid resolution to $N_d = \frac{d_p}{h} = 24$ in this regime without any significant change in the results. In all cases, Gunn's correlation predicts a larger value of the Nusselt number. Actually, Thiam et al. [136] showed that Gunn's correlation better fits the definition of the Nusselt number based on the fluid-phase averaged temperature (see Eq. (3.24)). Finally, the Nusselt number calculated from the log-linear regression on the bulk temperature profile reproduces very well that computed from the fluid phase heat balance. The deviation between the two estimates increases slightly at $Re_p = 10$, where neglecting axial conduction in the 1-D model is less justified, but the error bars of the two methods overlap in all cases. In the following, all Nusselt numbers will be computed using the interfacial heat flux $Q_{s \rightarrow f}^{(f)}$.

Different authors [120, 136] have noted the inconsistency to use a Nusselt number defined in terms of the bulk fluid temperature to model the interfacial heat transfer term given that the transported variable in the Euler-Euler model is the fluid-phase average temperature $\langle T^{(f)} \rangle$ (see Eq. (3.22)). As noted by Thiam et al. [136], the definitions (3.33) and (3.24) lead to the following relation

$$Nu_b (\langle T_b \rangle_m - T_s) = Nu_f (\langle T^{(f)} \rangle_m - T_s). \quad (3.37)$$

As mentioned earlier, the scaled temperature is statistically homogeneous in the thermally developed region, so that Eq. (3.37) can be recast as

$$\frac{Nu_b}{Nu_f} = \langle \theta^{(f)} \rangle_m = \langle \theta^{(f)} \rangle. \quad (3.38)$$

Therefore, the interphase heat transfer term in the Euler-Euler model should be more correctly closed as

$$q_{s \rightarrow f} = \frac{6\phi_s k_f}{d_p^2} Nu_b \frac{(T_s - \langle T^{(f)} \rangle)}{\langle \theta^{(f)} \rangle}. \quad (3.39)$$

In order to be consistent, not only Nu_b requires a closure but also the ratio $\frac{\text{Nu}_b}{\text{Nu}_f}$ or equivalently $\langle \theta^{(f)} \rangle$. In [120], Sun et al. derived a correlation for $\langle \theta^{(f)} \rangle$ as a function of Re_p and ϕ_s :

$$\langle \theta^{(f)} \rangle = 1 - 1.6\phi_s(1 - \phi_s) - 3(1 - \phi_s)\phi_s^4 \exp\left(-\text{Re}_p^{0.4} \phi_s\right). \quad (3.40)$$

In Figure 3.7, we plot the evolution of the ratio $\frac{\text{Nu}_f}{\text{Nu}_b}$ obtained from our PR-DNS data as a function of the volume fraction. It can be observed that this ratio deviates further from unity as the volume fraction increases and the Reynolds number decreases. Indeed, in viscous and dense regimes, the fluctuations of the streamwise velocity with respect to the fluid-phase averaged velocity are more significant, which results in larger differences between the bulk and the fluid-phase averaged temperatures. The comparison with the data of Thiam et al. [136] is satisfactory, except at low Reynolds number and high solid volume fraction where a significant difference is observed. These cases correspond to regimes where thermal saturation occurs very fast, which can lead to some imprecision in the results, as discussed earlier. We also plot for comparison the correlation of Sun et al. [120] (Eq. (3.40)) which is equivalent to the ratio of the Nusselt numbers. The global shape of the curves is recovered by our PR-DNS data but the discrepancy is significant. Actually, Sun et al. [120] derived Eq. (3.40) from PR-DNS data at $\text{Pr} = 0.7$ while we used $\text{Pr} = 1$ in our own simulations, which might partly explain the disagreement.

3.3.4 Pseudo-turbulent heat flux

Beside the interfacial heat flux, the pseudo-turbulent heat flux (PTHF) term in Eq. (3.7) also requires closure modeling. This term amounts for the heat transported by the covariance of the temperature and velocity fields at the micro-scale. Thiam et al. [136] proposed a closure for the PTHF by stating that

$$\langle (T \mathbf{u})^{(f)} \rangle = \mathcal{T}_b \cdot \langle \mathbf{u}^{(f)} \rangle, \quad (3.41)$$

where $\mathcal{T}_b$ is a tensor defined by

$$\mathcal{T}_{b,ij} = \frac{\langle (T u_i)^{(f)} \rangle}{\| \langle \mathbf{u}^{(f)} \rangle \|^2} \langle u_j^{(f)} \rangle. \quad (3.42)$$

In our simulations, the mean flow is aligned with the z direction so that $\langle \mathbf{u}^{(f)} \rangle = \langle u_z^{(f)} \rangle \mathbf{e}_z$. Consequently, the tensor $\mathcal{T}_b$ reduces to a single scalar component $\mathcal{T}_{b,zz}$,

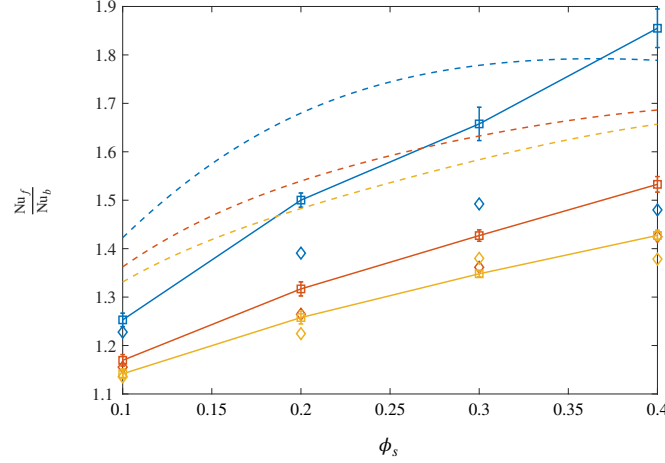


Figure 3.7: Evolution of the Nusselt numbers ratio with the solid volume fraction at $Re_p = 10$ ($\square$), $Re_p = 50$ ($\square$) and $Re_p = 100$ ($\square$). Our results are compared with the data of Thiam et al. [136] ($\diamond$, $\diamond$, $\diamond$) and with the correlation of Sun et al. [120] given by Eq. (3.40) ($-$, $-$ and $-$, respectively).

which corresponds to the bulk temperature T_b :

$$\tau_{b,zz} = \frac{\langle (T u_z)^{(f)} \rangle}{\langle u_z^{(f)} \rangle} = \langle T_b \rangle \quad (3.43)$$

and Eq. (3.41) takes the simpler form

$$\langle (T \mathbf{u})^{(f)} \rangle = \langle (T u_z)^{(f)} \rangle \mathbf{e}_z = \langle T_b \rangle \langle u_z^{(f)} \rangle \mathbf{e}_z. \quad (3.44)$$

It follows from Eq. (3.44) that the streamwise component of the temperature-velocity covariance can be written as

$$\langle (T' u_z')^{(f)} \rangle = \langle (T u_z)^{(f)} \rangle - \langle T^{(f)} \rangle \langle u_z^{(f)} \rangle = (\langle T_b \rangle - \langle T^{(f)} \rangle) \langle u_z^{(f)} \rangle. \quad (3.45)$$

As mentioned earlier, $\langle T_b \rangle$ is not a solution field of the Euler-Euler model. From Eq. (3.38), the difference between the bulk and the fluid-phase averaged temperature can be recast as

$$\langle T^{(f)} \rangle - \langle T_b \rangle = \left(\frac{Nu_f}{Nu_b} - 1 \right) (T_s - \langle T^{(f)} \rangle), \quad (3.46)$$

which lead Thiam et al. [136] to propose the following closure:

$$\langle (T' u_z')^{(f)} \rangle = - \left(\frac{\text{Nu}_f}{\text{Nu}_b} - 1 \right) (T_s - \langle T^{(f)} \rangle) \langle u_z^{(f)} \rangle. \quad (3.47)$$

Hence, the PTHF is closed if a relation is provided for the Nusselt numbers ratio, i.e. for $\langle \theta^{(f)} \rangle$. It must be noted that $\langle (T' u_z')^{(f)} \rangle$ is not homogenous since $\langle T^{(f)} \rangle$ varies along the streamwise direction. In a recent study, Sun et al. [121] showed that the PTHF can be written as

$$\langle (T' u_z')^{(f)} \rangle(z) = \langle (\theta u_z')^{(f)} \rangle (\langle T_b \rangle(z) - T_s), \quad (3.48)$$

where $\langle (\theta u_z')^{(f)} \rangle$ is a homogeneous quantity that we will refer to as the scaled pseudo-turbulent heat flux. As mentioned by the authors, Eq. (3.48) indicates that the variation of the PTHF along the streamwise direction is only due to the inhomogeneity of the bulk fluid temperature. Figure 3.8 shows the streamwise profile of $\langle (\theta u_z')^{(f)} \rangle$ obtained from our simulations at $\text{Re}_p = 50$ and $\phi_s = (0.1, 0.2, 0.3, 0.4)$, confirming that $\langle (\theta u_z')^{(f)} \rangle$ is homogeneous in the thermally developed region between $z_a = 2d_p$ and $z_b = 10d_p$. In the same study [121], a relation is proposed for the scaled PTHF as

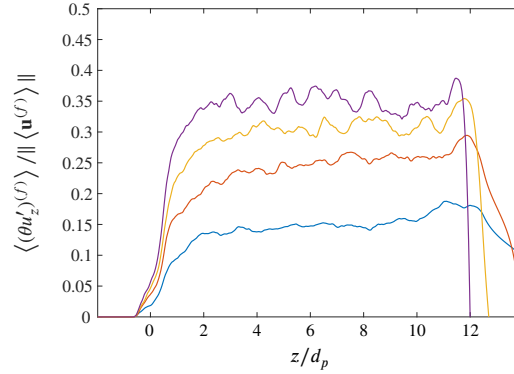


Figure 3.8: Streamwise profile of the scaled pseudo-turbulent heat flux at $(\text{Re}_p, \text{Pr}) = (50, 1)$ and for the volume fractions $\phi_s = 0.10$ (—), $\phi_s = 0.20$ (—), $\phi_s = 0.30$ (—) and $\phi_s = 0.40$ (—).

a function of the Reynolds number and the solid volume fraction:

$$\langle (\theta u_z')^{(f)} \rangle = (0.2 + 1.2\phi_s - 1.24\phi_s^2) \exp(-0.002 \text{Re}_p) \|\langle \mathbf{u}^{(f)} \rangle\|. \quad (3.49)$$

By combination of Eqs. (3.47) and (3.48), $\langle (u_z \theta)^{(f)} \rangle$ can be expressed as

$$\langle (\theta u'_z)^{(f)} \rangle = \left(1 - \frac{\text{Nu}_b}{\text{Nu}_f}\right) \langle u_z^{(f)} \rangle = (1 - \langle \theta^{(f)} \rangle) \langle u_z^{(f)} \rangle, \quad (3.50)$$

showing that $\langle (\theta u'_z)^{(f)} \rangle$ and $\langle \theta^{(f)} \rangle$ are univocally related. In Figure 3.9, we compare the mean values of $\langle (\theta u'_z)^{(f)} \rangle$ in the thermally developed region to the values obtained with the closure proposed by Thiam et al. [136] (Eq. (3.50)) using the actual ratio of Nusselt numbers obtained from our PR-DNS data. The agreement is very good, for all the Reynolds numbers and volume fractions we investigated. In the same figure, we plot the values obtained for $\langle (\theta u'_z)^{(f)} \rangle$ using the correlation given by Eq. (3.49) and using the closure (3.50) but with $\langle \theta^{(f)} \rangle$ given by the correlation of Sun et al. [120] (Eq. (3.40)). The two correlations yield very similar results at $\text{Re}_p = 100$ but they deviate more significantly at lower Reynolds number. Again, the global shape of the curve is recovered by our results but there is a clear divergence that we cannot explain so far.

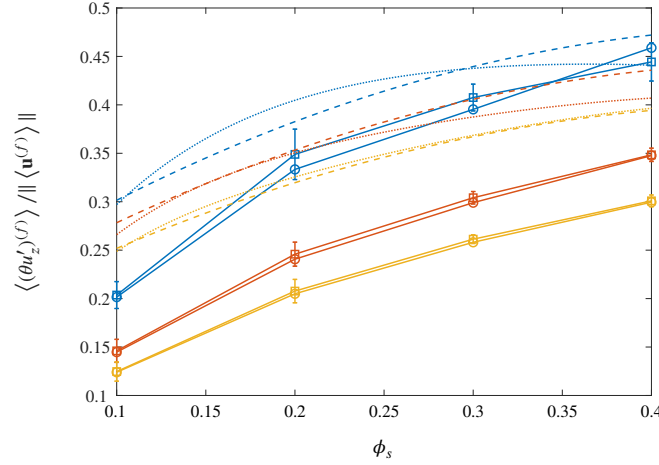


Figure 3.9: Evolution of the scaled pseudo-turbulent heat flux with the solid volume fraction at $\text{Re}_p = 10$ (blue), $\text{Re}_p = 50$ (red) and $\text{Re}_p = 100$ (yellow). The PTHF has been evaluated directly from PR-DNS (squares) and using the closure (3.50) based on the ratio of Nusselt numbers obtained from PR-DNS (circles). Our results are compared with the correlation (3.49) of Sun et al. [120] (dashed lines) and with the closure (3.50) using the correlation (3.40) to evaluate $\langle \theta^{(f)} \rangle$ (dotted lines).

3.3.5 Heat flux distribution

We now consider the distribution of the fluid-particle heat flux Q_p among the particles contained inside the control volume. On the left of Figure 3.10, we present the distribution of the normalized heat flux

$$Q_p^* = \frac{Q_p d_p}{S_p k_f (T_s - \langle T_b \rangle_m)} \quad (3.51)$$

for the different flow regimes. It comes from the definition (3.51) that the average of Q_p^* over all the particles contained in the control volume corresponds to the solid

phase evaluation of Nu_b since $\frac{\langle Q_p \rangle}{S_p} = \frac{q_{s \rightarrow f}^{(DNS)}}{a_p}$, where $\langle Q_p \rangle = \frac{1}{N_p} \sum_{k=1}^{N_p^{(V)}} Q_p^{(k)}$. The mean Nusselt number evaluated from the fluid phase heat balance is also indicated in Figure 3.10 (vertical dashed lines). The results show the large dispersion of the fluid-particle heat flux around the mean value. In addition, the distributions have a highly skewed shape and the skewness increases as Re_p decreases and ϕ_s increases. This finding is consistent with the discussions above regarding the very rapid thermal saturation of the flow in viscous and dense regimes. In those regimes, only the first rows of particles participate to most of the heat transfer leading to many occurrences of near zero fluxes in the rest of the bed. Consequently, the shape of the distribution of the fluid-particle heat flux is highly dependent on the streamwise dimension of the control volume.

To overcome this problem, we introduce the particle Nusselt number,

$$Nu_b^{(p)} = \frac{Q_p d_p}{S_p k_f (T_s - \langle T_b(z_p) \rangle)} \quad (3.52)$$

where the temperature difference at the denominator is based on the local bulk temperature evaluated at the streamwise position of the particle. Figure 3.11 compares the streamwise distribution of the normalized heat flux and the particle Nusselt number at $(Re_p, \phi_s) = (50, 0.20)$ (slow thermal saturation) and $(Re_p, \phi_s) = (10, 0.40)$ (rapid thermal saturation). As expected, the values of Q_p^* are not homogeneously distributed along the bed, with larger values encountered at the beginning of the bed and close to zero fluxes at the end of the bed. This pattern is much more pronounced at $(Re_p, \phi_s) = (10, 0.40)$. Conversely, $Nu_b^{(p)}$ is fairly homogeneously distributed along the bed in both cases. One can just notice that the occurrence of very large values increases at the end of the bed as both the numerator and the denominator in Eq. (3.52) are approaching zero, leading to more variability. The distribution of $Nu_b^{(p)}$ in the different

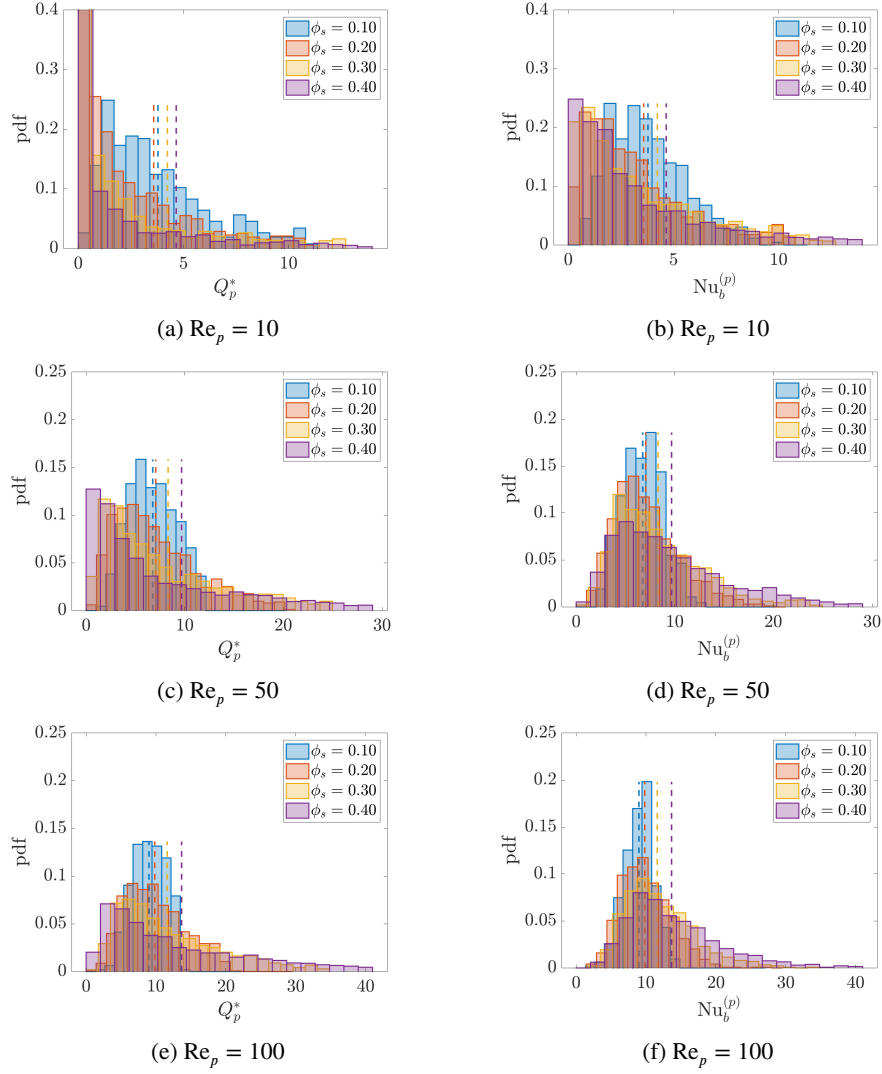


Figure 3.10: Distribution of the normalized fluid-particle heat flux (left) and the particle Nusselt number (right) among the particles contained in the control volume bounded by $z_a = 2d_p$ and $z_b = 10d_p$. The vertical dashed lines indicate the mean Nusselt number at the corresponding Reynolds number and $\phi_s = 0.10$ (---), $\phi_s = 0.20$ (---), $\phi_s = 0.30$ (---), $\phi_s = 0.40$ (---). At $(Re_p, \phi_s) = (10, 0.40)$ (top left), the distribution of Q_p^* has been truncated vertically for readability reasons.

flow regimes is presented on the right of Figure 3.10. The skewness of the distributions is still pronounced at low Re_p and high ϕ_s but overall weaker compared to Q_p^* and the occurrence of near zero values is strongly reduced. From Figure 3.11d, it can be inferred that the asymmetry in the distribution of $\text{Nu}_b^{(p)}$ at $(\text{Re}_p, \phi_s) = (10, 0.40)$ is not caused by thermal saturation but is rather related to the fact that, at a given streamwise location, many particles have a particle Nusselt number lower than the mean value and only a few particles show very high $\text{Nu}_b^{(p)}$ values. Therefore, conversely to Q_p^* , the distribution of $\text{Nu}_b^{(p)}$ should not be much sensitive to the streamwise dimension of the control volume. This finding is further confirmed by Figure 3.12 where we compare the distributions of $\text{Nu}_b^{(p)}$ and Q_p^* at $(\text{Re}_p, \phi_s) = (10, 0.40)$ in the control volume bounded by $z_a = 2d_p$ and $z_b = 10d_p$ and in that bounded by $z_a = 2d_p$ and $z_b = 6d_p$. While the distribution of Q_p^* changes significantly when the length of the control volume is reduced, the distribution of $\text{Nu}_b^{(p)}$ remains essentially unchanged.

3.3.6 Correlation with microstructure characteristic quantities

As a final investigation, we examine the possibly existing correlations between the interfacial heat flux and the microstructure characteristic quantities introduced in Chapter 2. We showed that the distribution of the particle Nusselt number $\text{Nu}_b^{(p)}$ is statistically homogeneous in the streamwise direction. Hence, it should be a better candidate than Q_p^* since the latter is impacted by the thermal saturation. Since we are no longer in a tri-periodic domain, we have to restrain our analysis to the part of the bed where microstructure characteristic quantities can be evaluated without being affected by the inlet and outlet of the bed. Therefore, the control volume is here bounded by $z_a = 4d_p$ and $z_b = 8d_p$. We show in Figure 3.13 the scatter plots between $\text{Nu}_b^{(p)}$ and the streamwise components of $\mathbf{K}_p$ and β_p at $(\text{Re}_p, \phi_s) = (50, 0.30)$. The correlation coefficients between $\text{Nu}_b^{(p)}$ and $K_{p,z}$ and between $\text{Nu}_b^{(p)}$ and $\beta_{p,z}$ are respectively $\rho = 0.075$ and $\rho = -0.30$. Hence, it appears that the correlations between $\text{Nu}_b^{(p)}$ and the microstructure characteristic quantities retained in the model in Chapter 2 are weak, but the trend is similar to what we observed for the streamwise component of the fluid-particle force: a negative correlation with $\beta_{p,z}$, meaning that a local alignment of the particles with the flow ($\beta_{p,z} > 0$) leads to a reduced heat flux; and a positive correlation with $K_{p,z}$, meaning that a microstructure that is locally oriented upstream ($K_{p,z} < 0$) induces a shielding effect also for the interfacial heat flux. Although not shown here, we mention that the correlations between $\text{Nu}_b^{(p)}$ and the transverse components of $\mathbf{K}_p$ and β_p are virtually zero. Obviously, this study is very preliminary, and we should further investigate the other flow regimes and the possible correlations with other microstructure

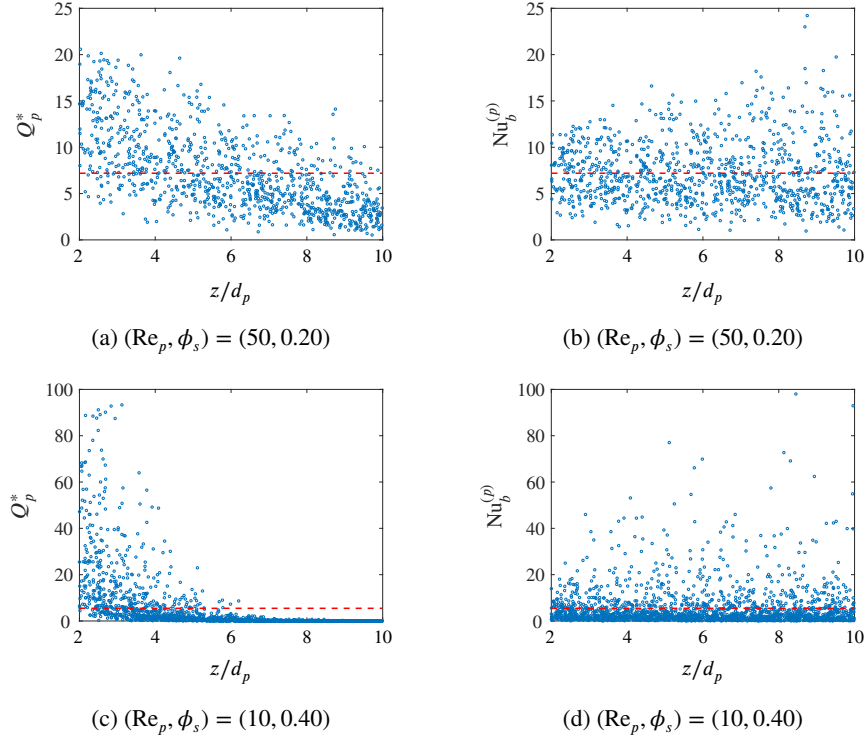


Figure 3.11: Streamwise distribution of the normalized fluid-particle heat flux (left) and the particle Nusselt number (right) at $(Re_p, \phi_s) = (50, 0.20)$ (top) and $(Re_p, \phi_s) = (10, 0.40)$ (bottom). The dashed red lines (---) indicates the mean Nusselt number Nu_b of the corresponding regime.

characteristic quantities. The parameters in the definitions of the microstructure-based tensors introduced in Chapter 2 may also have to be adapted to the heat transfer problem.

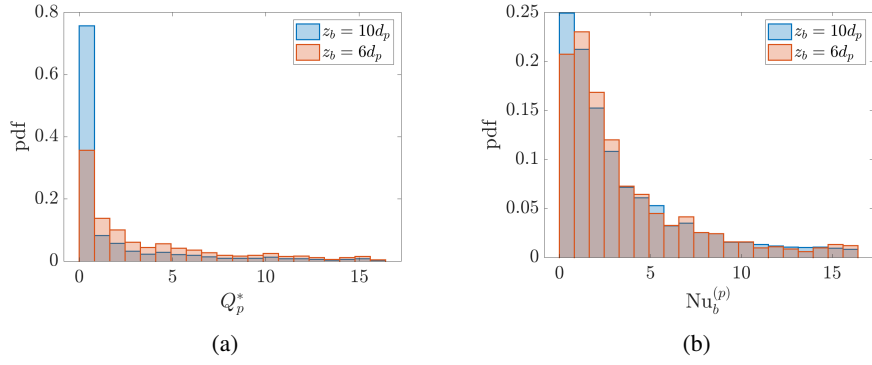


Figure 3.12: Distribution of the normalized fluid-particle heat flux (left) and the particle Nusselt number (right) among the particles contained in the control volume bounded by $z_a = 2d_p$ and $z_b = 10d_p$ (blue) or $z_b = 6d_p$ (red) at $(Re_p, \phi_s) = (10, 0.40)$.

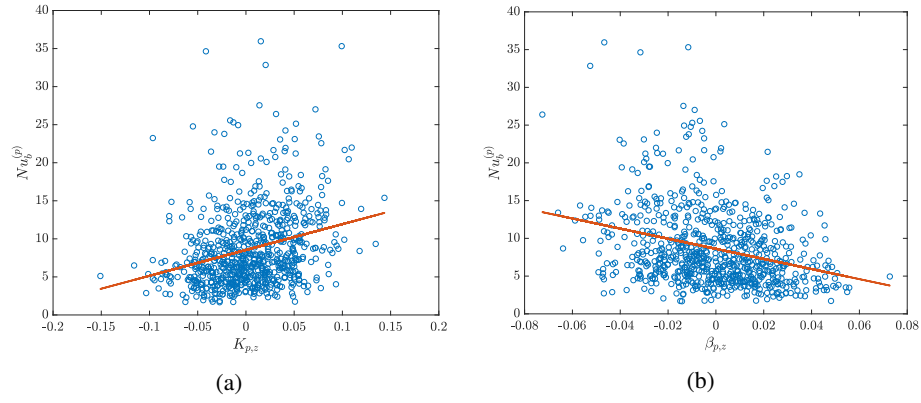


Figure 3.13: Scatter plots between $Nu_b^{(b)}$ and $K_{p,z}$ (left) and between $Nu_b^{(b)}$ and $\beta_{p,z}$ (right) at $(Re_p, \phi_s) = (50, 0.30)$.

3.4 Conclusions

In this study, we performed fully resolved simulations of the flow past fixed arrays of spheres with heat transfer using the DF-IBM described in Chapter 1. Our PR-DNS data have been used to evaluate unclosed terms in the Euler-Euler energy equation, namely the interfacial heat flux and the pseudo-turbulent heat flux. The interfacial heat flux is classically closed by means of a Nusselt number characterizing the heat transfer between the solid and the fluid phases. Several correlations have been proposed in the literature, either obtained experimentally ([53]) or numerically ([25, 134]). Our results agree reasonably well with the most recent correlations, although some deviations are observed in very inertial and dilute regimes as well as in regimes where thermal saturation occurs very fast (i.e. dense and viscous regimes). As noted in previous studies [120, 136], there is some inconsistency in using a Nusselt number based on the bulk temperature $\langle T_b \rangle$ in the Euler-Euler approach since the transported variable is the fluid-phase averaged temperature $\langle T^{(f)} \rangle$. To overcome this problem, Sun et al. [120] proposed a correlation for the fluid-phase average of the scaled temperature $\langle \theta^{(f)} \rangle$ which corresponds to the ratio of the Nusselt numbers based on $\langle T_b \rangle$ and $\langle T^{(f)} \rangle$, respectively. Our results confirm that both the ratio of the Nusselt numbers and the Nusselt number itself are homogeneous in the thermally developed region of the flow. Thiam et al. [136] identified a link between the PTHF and the ratio of Nusselt numbers while Sun et al. [121] derived a correlation for the scaled PTHF $\langle (\theta u'_z)^{(f)} \rangle$. Only qualitative agreement is observed with Sun's correlation. Then, we studied the distribution of the fluid-particle heat flux among the particles immersed in the array. Thermal saturation induces strong asymmetry in the shape of the heat flux distributions and this effect is more pronounced as the Reynolds number decreases and the volume fraction increases. Finally, we also defined a particle Nusselt number based on the local bulk temperature to report statistics that are independent of the streamwise extent of the control volume. It appears that this quantity still presents some skewness but its distribution does not depend on the streamwise location. Finally, we tried to correlate the particle Nusselt number to the microstructure characteristic quantities retained in the model of the streamwise component of the fluid-particle force in Chapter 2 for the case $(\text{Re}_p, \phi_s) = (50, 0.30)$. Although this study was very preliminary, it was shown that the correlation coefficients were non-zero but much smaller than with the fluid-particle force. However, the same trends were observed regarding the sign of the correlations.

In the future, we should further investigate the relation between the interfacial fluid-particle heat flux and the local organization of the microstructure formed by the solid

particles. A possible alternative would be to compute a Nusselt number based on the locally averaged fluid-phase temperature, such as proposed by several authors [126, 38]. We also aim at reproducing the above simulations at different Pr values to assess more accurately the sensitivity of the Nusselt number ratio (and therefore the PTHF) to the Prandtl number. Finally, we should add natural convection effects and evaluate their impact on the interfacial heat flux and on the PTHF.

Particle resolved simulation of liquid-solid and gas-solid fluidized beds

4.1 Introduction

Since its commercialization in the 1920s for coal gasification, the fluidized bed technology has found applications in many industries, including the petrochemical, pharmaceutical and nuclear industries. The popularity of the fluidized bed stems from its unique properties in terms of solids mixing as well as heat and mass transfer efficiency thanks to high exchange surface areas and high relative velocities between the fluid and the solids. The establishment of the fluidized state comes from the macroscopic balance between the buoyancy force due to the bed weight and the drag force exerted by the incoming fluid. Although simple, this equilibrium leads to complex phenomena ranging from the homogeneous suspension to the turbulent and chaotic fluidization regime. In this chapter, we investigate through particle-resolved simulations the dynamics of liquid-solid and gas-solid fluidized beds. Liquid-solid fluidized beds are used in the industry as crystallizers, heat exchangers, or bio-reactors [32], among others. Gaseous fluidization is nowadays more commonly implemented. Typical applications of gas-solid fluidized beds include fluid catalytic cracking (FCC) reactors in the petroleum industry, ore roasting in metallurgy and drying of solids in the food industry [69]. Due to the moderate density ratio between the solid phase and the carrying fluid, the suspension of solid particles by a liquid usually results in a smooth expansion of the bed that is referred to as homogeneous or particulate fluidization. Put it another way, the

fairly large density of most liquids causes the damping of instabilities that could arise in the bed. Conversely, gas-solid fluidized beds are characterized by a large solid-fluid density ratio so that the inertia of the solid particles becomes significant. In addition, particle-particle collisions are expected to play a more important role in the bed dynamics in dense regimes. As a result, gaseous fluidization usually leads to the emergence of strong heterogeneities, namely bubbling and slugging phenomena and the formation of particle clusters.

Owing to their industrial importance, fluidized beds have been the subject of intense research. Numerical simulations based on the Euler-Euler (EE) or the Euler-Lagrange (EL) approaches are nowadays commonly used for the design, scale-up and operation of these technologies. However particle-resolved simulations of micro-scale fluidized beds are much less frequent. Kriebitzsch et al. [68] performed resolved simulations of a gas-solid fluidized bed and noted that drag laws used in EL methods underestimate significantly the actual fluid-particle force. In [75], Luo et al. simulated a pseudo 2-D shallow gas-solid fluidized bed using an IBM similar to ours. More recently, Ozel. et al [95] used a viscous penalty method [145] to simulate a liquid-solid fluidized bed and compared their results with the experimental data of Aguilar [1]. In [36], Esteghamatian et al. performed resolved simulations of a liquid-solid and a gas-solid fluidized bed and made a thorough comparison of their dynamics. These PR-DNS data were then compared to results obtained at the meso-scale using an Euler-Lagrange approach [34] and they were subsequently used to propose a stochastic formulation of the drag force [35]. Direct numerical simulations of the thermal problem in fluidized beds are even more scarce. Feng and Musong [45] first simulated the heat transfer in a liquid-solid fluidized bed containing 225 spherical particles. Recently, Euzenat [37] and Thiam [135] investigated in their respective theses the heat transfer in fluidized beds for larger particle systems.

This chapter is structured as follows. In Section 4.2, we recall the basics of fluidization theory. We then briefly introduce in Section 4.3 the statistical operators used in the chapter. As a preamble to fluidized beds, Section 4.4 is dedicated to the study of settling suspensions. In Section 4.5, we investigate in details the hydrodynamics and heat transfer of liquid-solid fluidized beds for different superficial velocities. Finally, Section 4.6 concerns gas-solid fluidized beds.

4.2 Fluidization theory

4.2.1 Minimum fluidization

Fluidization describes the pseudo-fluid state of a system of solid particles under the action of an upwardly moving fluid (gas or liquid). When a gas or a liquid flows vertically through a fixed bed of particles, a significant pressure drop is measured between the inlet and the outlet of the bed. When this pressure drop compensates the weight of the solid particles, the bed is said to be at minimum fluidization [48], which reads

$$-\frac{dp_t}{dz} = (\rho_s(1 - \phi_f) + \rho_f\phi_f)g, \quad (4.1)$$

where p_t is the total pressure and ϕ_f is the fluid volume fraction of the bed (or voidage). The dynamic pressure gradient is obtained by subtracting the hydrostatic contribution from Eq. (4.1), i.e.

$$-\frac{dp}{dz} = -\frac{dp_t}{dz} - \rho_f g = (1 - \phi_f)(\rho_s - \rho_f)g. \quad (4.2)$$

The contribution of the hydrostatic pressure gradient is negligible in gas-solid fluidized beds but it might be significant when a liquid is the carrying fluid. As illustrated in Figure 4.1, the pressure drop across the bed remains constant once the minimum fluidization point has been reached although the superficial velocity U_0 is further increased.

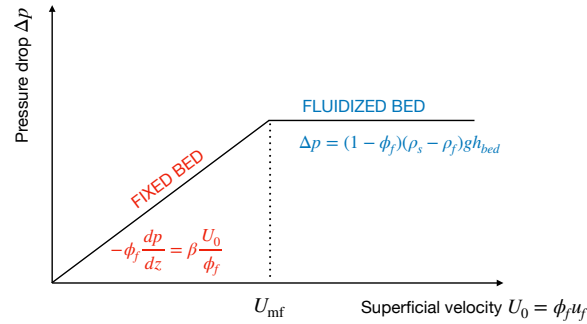


Figure 4.1: Pressure drop across the bed in the fixed bed and fluidized bed regimes.

The gradient of dynamic pressure can be related to the drag force as

$$-\phi_f \frac{dp}{dz} = \beta(u_f - u_s), \quad (4.3)$$

where β is the friction coefficient, while u_f and u_s correspond to the interstitial velocities of the fluid and solid phases, respectively. The particle Reynolds number in fluidization is usually defined in terms of the relative (or slip) velocity as

$$\text{Re}_p = \frac{\rho_f d_p \phi_f |u_f - u_s|}{\mu}, \quad (4.4)$$

with

$$u_f = \frac{U_0}{\phi_f}. \quad (4.5)$$

The friction coefficient β can be obtained from Ergun's correlation [33],

$$\beta = 150 \frac{(1 - \phi_f)^2 \mu}{\phi_f (\psi_s d_p)^2} + 1.75 \frac{\rho_f (1 - \phi_f)}{(\psi_s d_p)} |u_f - u_s|, \quad (4.6)$$

where ψ_s is the sphericity of the particles. In the present work, only perfect spheres are considered, so that $\psi_s = 1$.

At the onset of fluidization, the solid phase is at rest (i.e. $u_s = 0$) and $u_f = \frac{U_{mf}}{\phi_{f,mf}}$, where $\phi_{f,mf}$ and U_{mf} correspond to the voidage and superficial velocity at minimum fluidization. By combining Eqs. (4.1) and (4.3), we obtain a relation between U_{mf} and $\phi_{f,mf}$,

$$(1 - \phi_{f,mf})(\rho_s - \rho_f)g = \frac{\beta}{\phi_{f,mf}^2} U_{mf}. \quad (4.7)$$

Using the expression of the friction coefficient given by Eq. (4.6), Eq. (4.7) can be recast as

$$150A \text{Re}_{mf} + 1.75B \text{Re}_{p,mf}^2 = \text{Ga}, \quad (4.8)$$

where

$$\text{Re}_{mf} = \frac{\rho_f U_{mf} d_p}{\mu} \quad (4.9)$$

is the Reynolds number at minimum fluidization,

$$\text{Ga} = \frac{d_p^3 (\rho_s - \rho_f) \rho_f g}{\mu^2}, \quad (4.10)$$

is the Galileo (or Archimedes) number, and

$$A = \frac{(1 - \phi_{f,mf})}{\psi_s^2 \phi_{f,mf}^3} \quad (4.11)$$

and

$$B = \frac{1}{\psi_s \phi_{f,mf}^3} \quad (4.12)$$

are two constants. Hence, the minimum fluidization velocity can be calculated if we have an *a priori* estimate of $\phi_{f,mf}$; but the porosity at minimum fluidization is not always available and might vary significantly with the geometrical properties of the particles. However, Wen and Yu [152] noted that A and B take approximately constant values for different kinds of particles and for a large range of operating conditions. They suggest to use

$$A = 11 \quad \text{and} \quad B = 14. \quad (4.13)$$

Finally, the particle Reynolds number at minimum fluidization is obtained as

$$\text{Re}_{mf} = \sqrt{C_1^2 + C_2 \text{Ga}} - C_1, \quad (4.14)$$

where

$$C_1 = 33.7 \quad \text{and} \quad C_2 = 0.0408. \quad (4.15)$$

In the particular case of very small particles, i.e. small Reynolds number, the quadratic term in Eq. (4.8) becomes negligible. Then, using $A = 11$ as suggested by Wen and Yu [152], the minimum fluidization velocity can be estimated as

$$U_{mf} = \frac{d_p^2(\rho_s - \rho_f)g}{1650\mu}. \quad (4.16)$$

In comparison, the terminal settling velocity of a spherical particle in Stokes regime is given by

$$U_t = \frac{d_p^2(\rho_s - \rho_f)g}{18\mu}, \quad (4.17)$$

which gives a ratio $\frac{U_t}{U_{mf}} = \frac{1650}{18} \simeq 92$. This means that the flow rate velocity needed to fluidize a bed of particles in Stokes regimes is about 90 times smaller than the terminal velocity of an individual particle, also named entrainment velocity. This fundamental feature of the fluidized state comes from the largest friction coefficient β experienced by a sphere in a packed bed than that experienced by an isolated sphere. Oscillatory motions in fluidized beds originate from this change of resistance faced by the particles as they move upward in the vessel and then drop down when the flow can no longer compensate their weight. These oscillations also provide to fluidized bed reactors many of their interesting properties in terms of mixing, heat and mass transfer.

4.2.2 Terminal velocity and fluidization law

Outside the Stokes regime, the terminal velocity of a particle is obtained from the buoyancy-drag balance

$$\frac{\pi d_p^3}{6}(\rho_s - \rho_f)g = \frac{\pi d_p^2}{8}\rho_f U_t^2 C_{d,t}, \quad (4.18)$$

which yields

$$U_t = \sqrt{\frac{4}{3} \frac{(\rho_s - \rho_f)g d_p}{\rho_f C_{d,t}}}, \quad (4.19)$$

where the 'terminal' drag coefficient $C_{d,t}$ can be obtained from the Schiller-Naumann's equation [90]:

$$C_{d,t} = \begin{cases} \frac{24}{\text{Re}_t} (1 + 0.15 \text{Re}_t^{0.687}), & \text{Re}_t \leq 1000 \\ 0.44 & \text{Re}_t > 1000, \end{cases} \quad (4.20)$$

where the terminal Reynolds number is defined as

$$\text{Re}_t = \frac{\rho_f U_t d_p}{\mu}. \quad (4.21)$$

Since the drag coefficient is unknown a priori, Eq. (4.19) is solved iteratively: an initial guess is used for $C_{d,t}$, then U_t (and therefore Re_t) is obtained from Eq. (4.19), $C_{d,t}$ is updated from Eq. (4.20) and so on until two estimates of the terminal velocity are sufficiently close to consider that the procedure has converged. Eq. (4.19) can also be recast in terms of dimensionless quantities as

$$\text{Ga} = \frac{3}{4} \text{Re}_t^2 C_{d,t}, \quad (4.22)$$

which shows that the Galileo number and the terminal Reynolds number carry essentially the same information.

The fluidization law is the relationship between the superficial velocity U_0 and the porosity of the bed ϕ_f . By Galilean invariance it also provides the terminal settling velocity relatively to the fluid of a suspension of solid particles with the same void fraction. In homogeneous liquid-solid fluidization, Richardson-Zaki's law [104] postulates that the superficial velocity evolves linearly with the void fraction in a log-log scale, which reads

$$\frac{U_0}{U_{0,\infty}} = \phi_f^n, \quad (4.23)$$

where $U_{0,\infty}$ corresponds to the extrapolation of the superficial velocity at infinite dilution, i.e. at $\phi_f = 1$. In their original work [104], Richardson and Zaki set $U_{0,\infty} = U_t$ and they expressed the exponent n as a piecewise function of the terminal Reynolds number:

$$n = \begin{cases} 4.65 & \text{Re}_t < 0.2 \\ 4.4 \text{Re}_t^{-0.03} & 0.2 < \text{Re}_t < 1 \\ 4.45 \text{Re}_t^{-0.1} & 1 < \text{Re}_t < 500 \\ 2.4 & \text{Re}_t > 500 \end{cases} \quad (4.24)$$

Rowe [107], using the same data, proposed a single relationship for the entire range of terminal Reynolds number values:

$$\frac{4.7 - n}{n - 2.35} = 0.175 \text{Re}_t^{0.75}. \quad (4.25)$$

Khan and Richardson [67] later suggested a relation involving the Galileo number where n is determined by the following relation,

$$\frac{4.8 - n}{n - 2.4} = 0.043 \text{Ga}^{0.57}. \quad (4.26)$$

The same authors investigated the influence of the wall confinements effects on the value of $U_{0,\infty}$ and proposed the following relation,

$$\frac{U_{0,\infty}}{U_t} = 1 - 1.15 \left(\frac{d_p}{D} \right)^{0.6}, \quad (4.27)$$

where D is the diameter of the container. Eq. (4.27) indicates that the presence of walls will induce an entrainment of the solid particles at a lower velocity compared to the unbounded case. However, it has been reported in the literature [27, 40] that the extrapolation of the superficial velocity at infinite dilution can be lower than the terminal velocity, even in the absence of wall confinement effects. To be clear, the entrainment velocity is still given by U_t (in the absence of walls), but outside the very dilute regime ($\phi_f \lesssim 0.85 \dots 0.95$), the extrapolation of the (ϕ_f, U_0) curve to $\phi_f = 1$ yields a value lower than U_t . This results in a break of the straight line and a change of slope beyond a critical porosity, as illustrated in Figure 4.2. A model with two straight lines has been proposed by Rapagna et al. [103] in order to represent the two regimes, although the same authors mentioned that the high voidage region can be fitted to a quadratic curve. Another class of correlations have been proposed, where the explicit computation of the terminal Reynolds number is not required. They are mostly based

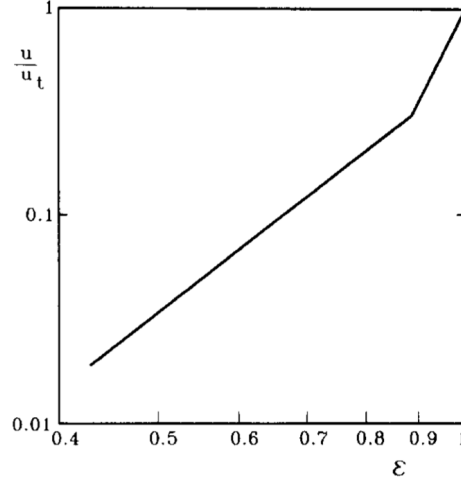


Figure 4.2: Bed expansion with a change in the slope of the fluidization law (reproduced from [27]¹).

on the original relation of Ramamurthy and Subbaraju [102]:

$$\begin{aligned}
 \frac{Ga}{18 \text{Re}_p} &= \Phi^{1.55} & Ga < 18 \\
 \frac{Ga}{13 \text{Re}_p^{1.4}} &= \Phi^{2.21} & 18 < Ga < 1 \times 10^5 \\
 \frac{3 Ga}{\text{Re}_p^2} &= \Phi^{3.21} & Ga > 1 \times 10^5,
 \end{aligned} \tag{4.28}$$

with $\Phi = (1 - 1.21(1 - \phi_f)^{2/3})^{-1}$.

Additional details about the hydrodynamics of homogeneous liquid-solid fluidization can be found in the review paper of Di Felice [27].

4.3 Statistical operators

We introduce here the notations used in this chapter for the different statistical operators.

¹Note that the void fraction is noted ϵ here.

For a Lagrangian quantity Ψ , its instantaneous arithmetic average over the ensemble of N_p particles is noted

$$\langle \Psi \rangle(t) = \frac{1}{N_p} \sum_{k=1}^{N_p} \Psi^{(k)}. \quad (4.29)$$

The fluctuation of Ψ is defined as

$$\Psi'(t) = \Psi(t) - \langle \Psi \rangle_t \quad (4.30)$$

where $\langle \Psi \rangle_t$ is the arithmetic average of Ψ over the N_p particle which has been further averaged in time at pseudo-steady state and for sufficiently long times. Hence, $\langle \Psi \rangle_t$ corresponds to the true ensemble average of Ψ for a large number of flow realizations. The variance of Ψ is then obtained as $\langle \Psi'^2 \rangle_t$.

For an Eulerian quantity ψ , its fluid-phase average is defined as

$$\langle \psi \rangle_f(t) = \frac{1}{V_f} \int_{V_f} \psi(\mathbf{x}, t) dV = \frac{\int_V \chi_f(\mathbf{x}, t) \psi(\mathbf{x}, t) dV}{\int_V \chi_f(\mathbf{x}, t) dV} \quad (4.31)$$

where V_f is volume occupied by the fluid and χ_f is the fluid phase indicator function. We also define the average of ψ over the cross-section occupied by the fluid at a streamwise position z as

$$\langle \psi \rangle_f(z, t) = \frac{1}{S_f} \int_{S_f(z)} \psi(\mathbf{x}, t) dV = \frac{\int_{S(z)} \chi_f(\mathbf{x}, t) \psi(\mathbf{x}, t) dS}{\int_{S(z)} \chi_f(\mathbf{x}, t) dS}. \quad (4.32)$$

Finally, we also define the time average of ψ over the time interval $[t_i, t_e]$ as

$$\overline{\psi}^{[t_i, t_e]} = \frac{1}{(t_e - t_i)} \int_{t_i}^{t_e} \psi(t) dt. \quad (4.33)$$

When the time average is computed over a long time interval at pseudo steady-state, we will omit the time interval in the superscript and simply write $\overline{\psi}$.

4.4 Hindered settling of a suspension of spherical particles

Let us first consider the hindered settling of N_p particles under the action of gravity in a three-dimensional periodic domain. An adverse pressure gradient is imposed in the

vertical direction z to cancel the net fluid flow rate, i.e. $\langle u_z \rangle_f = 0$. The settling velocity U_s of the suspension is defined as the time-average of the mean vertical velocity component of the solid particles when the flow has reached statistical steady state, i.e.

$$U_s = \langle u_{p,z} \rangle_t. \quad (4.34)$$

As mentioned earlier, this problem is identical, by Galilean invariance, to the fluidization of solid particles at a superficial velocity $U_0 = U_s$. The present simulations are performed in a three-dimensional periodic box with size $L = 12d_p$ containing $N_p = (50, 100, 200, 500, 1000)$ particles. The Galileo number is $Ga = 3930$, the density ratio is $\rho_r = 2.5$ and the estimated terminal Reynolds number is $Re_t = 61.6$. Regarding collision parameters, the normal and tangential restitution coefficients are set equal to $e_n = 0.97$ and $e_t = 0.39$ and the Coulomb's friction coefficient is set to $\mu_c = 0.4$. The grid resolution is $d_p = \frac{256}{12} \simeq 21.3h$ and the time step is set to $\Delta t = 2.88 \times 10^{-3} \frac{d_p}{U_c}$, where U_c is the characteristic velocity, defined as

$$U_c = \sqrt{\frac{4}{3} \frac{(\rho_s - \rho_f)gd_p}{\rho_f}}. \quad (4.35)$$

Let us also mention that the Reynolds number Re_c based on the characteristic velocity defined by Eq. (4.35) is linked to the Galileo number by the relation

$$Re_c^2 = \frac{4}{3} Ga, \quad (4.36)$$

which gives $Re_c = 72.4$. Figure 4.3 shows the magnitude of the velocity field for $N_p = 500$ settling particles (i.e. $\phi_s = 0.152$). Particles are homogeneously distributed in the domain and there is no observable clustering of particles nor large bubbles, so that one can compare this sedimentation to a homogeneous liquid-solid fluidization (e.g. such as small glass beads fluidized in water). Since the problem is statistically symmetric in the x and y directions, the following statistics will only be reported in the transverse direction x and the vertical direction z .

Figure 4.4a shows the evolution of the mean vertical velocity component of the solid particles as a function of the dimensionless time $t^* = \frac{tU_c}{d_p}$ for different solid volume fractions. As expected, the settling velocity of the suspension decreases (in absolute value) when the particles loading increases. Figure 4.4b confirms that the average transverse velocity component of the particles is zero on average (not net lateral motion). Figures 4.4c and 4.4d present the time evolution of the standard deviation of the vertical and transverse particle velocity components, respectively. First, it can be

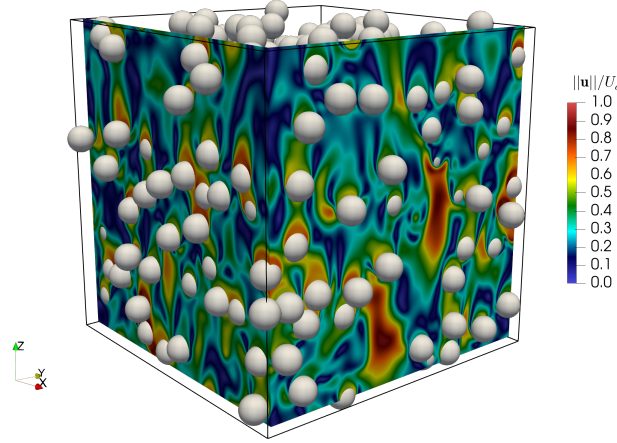


Figure 4.3: Hindered settling of $N_p = 500$ particles in a periodic box at $(\text{Ga}, \rho_r, \phi_s) = (3930, 2.5, 0.152)$: normalized velocity field magnitude.

observed that, while the mean of the vertical velocity component converges quickly to its steady-state value, this is not the case for the standard deviation, especially at low solid volume fraction. Besides, the level of fluctuations in the vertical velocity component seems little affected by the concentration in solid particles. In the transverse direction, Figure 4.4d shows that the level of fluctuations is similar for $\phi_s = 0.152$, 0.212 and 0.303, but it decreases significantly in the very dilute regimes. Particle-particle collisions allow the transfer of momentum between the vertical and transverse components of the velocity and their rarefaction in the dilute regime can explain this decrease in the intensity of particles lateral motion. However, the level of fluctuations in the transverse direction is always lower than in the vertical direction, showing the importance of vertical particle-wake interactions in the dynamics of the settling.

The settling velocity U_s was estimated from our PR-DNS data by taking the time average of $\langle u_{p,z} \rangle$ (see Eq. (4.34)) in the interval $t^* \in [30, 70]$ and the results are reported in Figure 4.5 as a function of the void fraction. Our results are also compared to the values obtained using the aforementioned fluidization law correlations (here used to evaluate U_s). The relations based on Richardson and Zaki's [104] law given by Eq. (4.23) correspond to straight lines in a log-log diagram and yield very similar results (they only differ in the value of the slope) while Ramamurthy and Subbaraju's

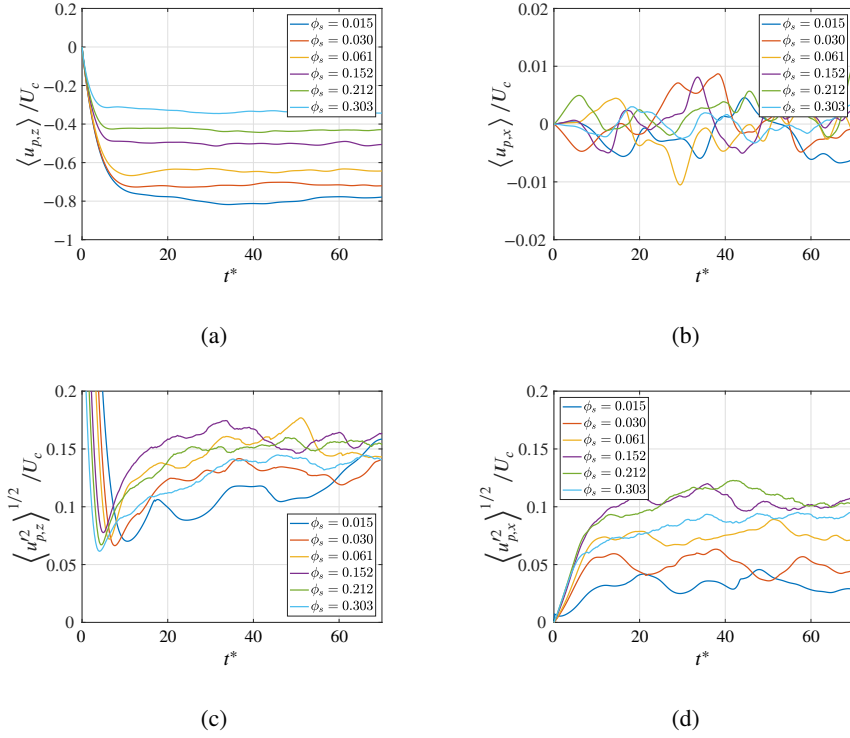


Figure 4.4: Hindered settling of a suspension of spherical particles at $(\text{Ga}, \rho_r) = (3930, 2.5)$: time evolution of (a) the mean vertical velocity, (b) the mean transverse velocity, (c) the standard deviation of the vertical velocity and (d) the standard deviation of the transverse velocity for different solid fractions.

relation [102] is slightly concave and predicts significantly lower settling velocities at a given voidage. It can be observed that our results do not reproduce a straight line over the whole range of void fractions. Actually, our (ϕ_f, U_s) curve seems to reproduce approximately the two-regimes behavior detailed earlier (see Figure 4.2). In the first part, between $\phi_f = 0.7$ and $\phi_f = 0.94$, the settling velocity follows a law similar to Eq. (4.23) but with a significantly lower slope ($n \simeq 2.15$ vs. 2.95 from Eq. (4.24)) and the extrapolation of the straight line to $\phi_f = 1$ returns a settling velocity at infinite dilution well below U_t . In the second part, between $\phi_f = 0.94$ and $\phi_f = 0.985$ (i.e. high voidage regime), the curve is becoming concave and it converges towards U_t for $\phi_f \rightarrow 1$.

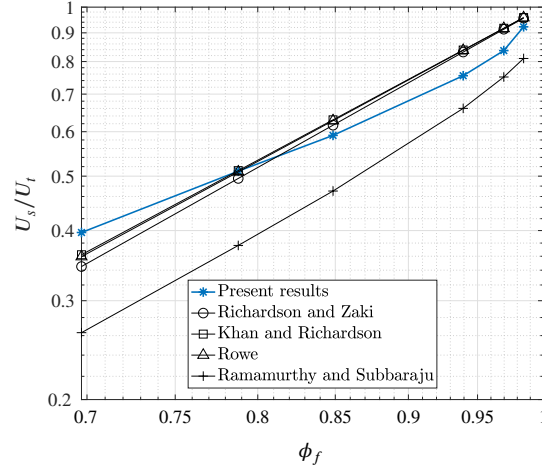


Figure 4.5: Suspension settling velocity as a function of the void fraction: comparison between our PR-DNS results and the correlations proposed by Richardson and Zaki [104], Khan and Richardson [67], Rowe [107] and Ramamurthy and Subbaraju [102]

The case with $N_p = 700$ settling particles (i.e. $\phi_s = 0.212$) has been simulated for different resolutions using $N_d = (10.67, 16, 21.33, 32)$ grid points per diameter. The three most resolved cases have been used to estimate the "exact" settling velocity $U_{s,\text{ref}}$ at infinite resolution using Richardson's extrapolation (see Eqs. (1.50) and (1.51)). The convergence of the error between the measured values of U_s and $U_{s,\text{ref}}$ is shown in Figure 4.6. The error decreases with a slope $p \simeq 1.3$, which corresponds to the "between first and second order" behavior of the IBM that was previously observed in Chapter 1.

As discussed earlier, the level of fluctuations in the particle velocity is higher in the vertical direction than in the transverse direction. This observation can be quantified by the anisotropy coefficient K_U , defined as

$$K_U = \sqrt{\frac{\langle u_{p,z}'^2 \rangle_t}{0.5 (\langle u_{p,x}'^2 \rangle_t + \langle u_{p,y}'^2 \rangle_t)}}. \quad (4.37)$$

As shown in Figure 4.7, the value taken by K_U is quite constant in the moderately dense regimes with $K_U \simeq 1.5$ between $\phi_f = 0.7$ and $\phi_f = 0.85$. This value is consistent with previously reported results for homogeneous liquid-solid fluidized beds, both

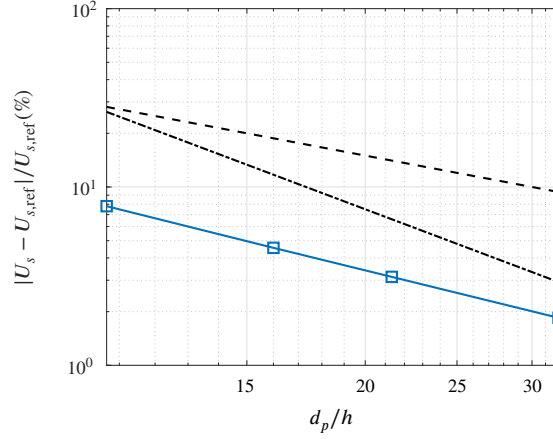


Figure 4.6: Convergence of the error on the settling velocity (■). The first (- -) and second (- · -) order convergence lines are shown for comparison

experimentally [1] and numerically [95]. Then, the anisotropy coefficient drastically increases with the void fraction. This behavior was also observed in [93] but for much lower Reynolds numbers. We also note that Ozel et al. [95] report constant values of K_U down to $\phi_f = 0.1$ in their resolved simulations of liquid-solid fluidized beds.

Finally, we verify that momentum conservation is globally satisfied by checking that the sum of the individual fluid-particle forces in the vertical direction compensates the pressure difference Δp applied in the vertical dimension of the domain (see momentum balance Eq. (B.2)). Figure 4.8 shows that momentum is well conserved as the mismatch between the total fluid-particle force and the pressure gradient is below 1 %, for all the volume fractions.

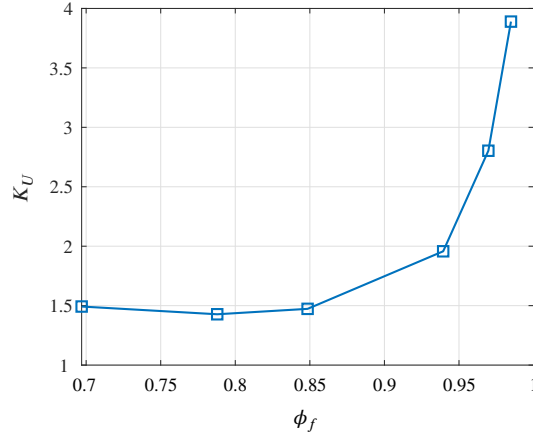


Figure 4.7: Evolution of the particle velocity anisotropy coefficient with the void fraction in a homogeneous settling suspension.

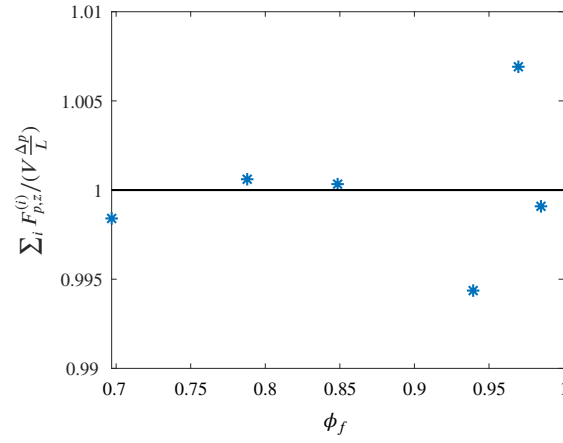


Figure 4.8: Ratio between the total fluid force experienced by the solid phase and the force exerted by the external pressure gradient over the volume of the domain.

4.5 Liquid-solid fluidized beds

We now investigate the dynamics of liquid-solid fluidized beds through particle resolved simulations. The Stokes number, defined as

$$\text{St}_k = \frac{\rho_s \phi_f |u_f - u_s| d_p}{18\mu} = \frac{\rho_s}{\rho_f} \frac{\text{Re}_p}{18}, \quad (4.38)$$

is the ratio between the particle relaxation time and the fluid relaxation time. In other words, the Stokes number characterizes the importance of the particles inertia. At low Stokes number, the particles face little resistance to the surrounding fluid flow and they adapt quickly to a change in the velocity field. Conversely, high Stokes numbers correspond to systems where the translational and rotational motions of the particles take a significant time before being modified by the flow. Liquid-solid fluidized beds are characterized by low to moderate solid-fluid density ratios, which yields Stokes numbers in the range $\mathcal{O}(1)$ to $\mathcal{O}(10)$. The rather limited inertia of the particles in the liquid generally leads to a homogeneous fluidization without major discontinuities in the bed (voids or clusters). In this section, we examine through PR-DNS the influence of the superficial velocity on the hydrodynamics of the bed and the dynamics of the particles. The thermal problem is also investigated. In the following, all ‘*’ quantities have been made dimensionless using the physical reference quantities. The reference length scale is the particle diameter d_p , the reference velocity scale is the superficial velocity U_0 and the reference time scale is thus given by d_p/U_0 .

4.5.1 Numerical set-up

The computational domain and the initial particle configuration used for the simulation of liquid-solid fluidized beds are displayed in Figure 4.9. The entrance of the domain is located at $z = -2d_p$ where the superficial velocity U_0 and the inlet temperature T_0 are prescribed. A virtual grid is located at $z = 0$ where particles are bouncing while the fluid is free to flow through. This prevents particles to reach the inlet of the domain and thereby allows the flow to develop over a distance equal to two particle diameters. The outlet of the domain is located at $z = z_{out} = 30d_p$ where we impose natural outflow boundary conditions. Periodic boundary conditions are used in the transverse directions. At initial time, the solid particles are randomly distributed between $z = 0$ and $z = 12d_p$. The physical and numerical parameters of the problem are detailed in Table. 4.1. We performed three distinct simulations at $\text{Re}_p = \frac{U_0 d_p}{\nu} = 20, 25$ and 30 by changing the superficial velocity imposed at the inflow while keeping all other physical parameters unchanged. The resolution was set to $N_d = \frac{d_p}{h} = 32$. This fine resolution

is justified by the thin thermal boundary layer at the surface of the particles for the fairly high Péclet numbers we considered. This feature makes the simulation of heat transfer in liquid fluidization particularly challenging. The Froude number in Table 4.1 is defined as $Fr = \frac{U_0^2}{gd_p}$. The Stokes number is also reported for convenience, although it must be noted that it is not an independent parameter as it is computed from the particle Reynolds number and the density ratio using Eq. (4.38). Obviously, the same remark holds for the Péclet number which is obtained from Re_p and Pr . To fix ideas, the set of parameters presented in Table 4.1 can be assimilated to the fluidization of small beads of steel in water at ambient temperature. From a computational perspective, each of these simulations ran for 7 days on 1024 processors (~ 172000 cpu.hours).

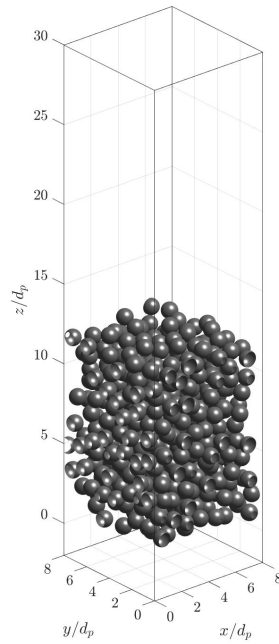


Figure 4.9: Computational domain and initial configuration of particles for the resolved simulation of liquid-solid fluidized beds.

Fluid density	ρ_f	1000	[kg/m ³]
Solids density	ρ_s	8000	[kg/m ³]
Fluid kinematic viscosity	ν	1×10^{-6}	[m ² /s]
Fluid thermal diffusivity	α	1.429×10^{-7}	[m ² /s]
Gravitational acceleration	g	9.81	[m/s ²]
Particle diameter	d_p	5×10^{-4}	[m]
Particle terminal velocity	U_t	0.2062	[m/s]
Minimum fluidization velocity	U_{mf}	0.0097	[m/s]
Superficial velocity	U_0	(0.04, 0.05, 0.06)	[m/s]
Ratio U_0/U_{mf}	U_0/U_{mf}	(4.12, 5.15, 6.19)	[-]
Number of particles	N_p	520	[-]
Normal restitution coefficient	e_n	0.97	[-]
Tangential restitution coefficient	e_t	0.39	[-]
Coulomb's friction coefficient	μ_c	0.1	[-]
Domain size	$L_x \times L_y \times L_z$	$8d_p \times 8d_p \times 32d_p$	[m ³]
Resolution	$N_d = \frac{d_p}{h}$	32	[-]
Time step	Δt	(5, 5, 4)	10^{-6} [s]
Density ratio	ρ_r	8	[-]
Particle Reynolds number	Re_p	(20, 25, 30)	[-]
Froude number	Fr	(0.33, 0.51, 0.74)	[-]
Stokes number	St_k	(8.89, 11.11, 13.33)	[-]
Prandtl number	Pr	7	[-]
Péclet number	Pe	(140, 175, 210)	[-]

Table 4.1: Resolved simulations of liquid-solid fluidized beds: physical and numerical parameters

4.5.2 Flow visualization, bed height and pressure drop

We show in Figure 4.10 the evolution of the liquid-solid fluidized bed with a superficial velocity $U_0 = 0.05$ [m/s] (i.e. $Re_p = 25$) at three distinct times. About a quarter of the total number of particles is visible on each frame since half of it has been removed for visualization reasons and the last quarter is located behind the median vertical plane. It can be observed that the bed expands homogeneously, confirming the smooth fluidization of the solid particles in a liquid at moderate Reynolds number.

Figure 4.11 shows the trajectories of four randomly chosen particles in a transverse and a vertical plane at $Re_p = 25$. These pictures show that the solid particles do not follow a pure random motion and are driven by large-scale structures. The anisotropy of particle motion is evidenced in Figure 4.11b where particles show larger displacements in the vertical direction. In the transverse direction, conversely, particle trajectories are isotropic, as expected. Again, given the statistical equivalence between the transverse directions x and y , particle statistics will only be reported in the z and x directions.

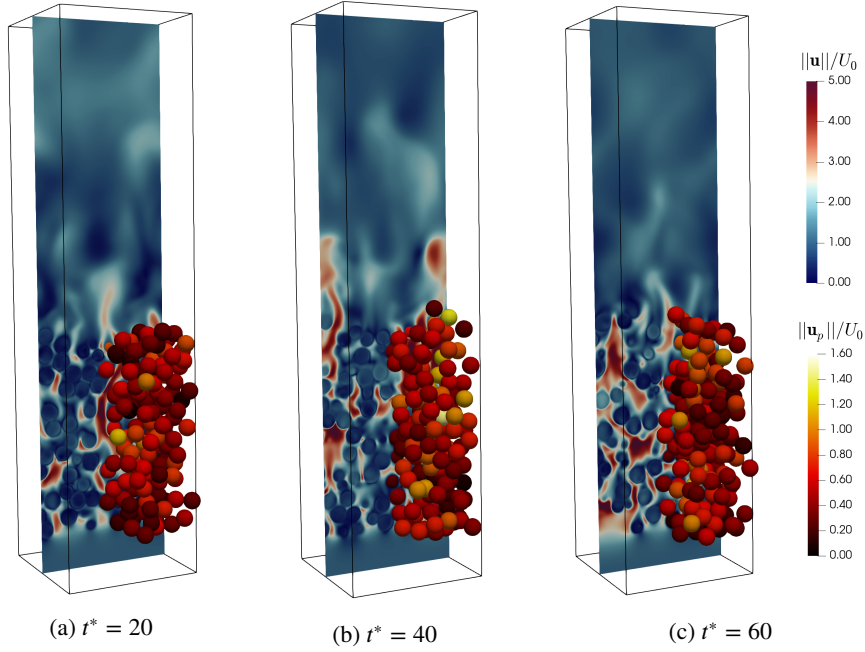


Figure 4.10: Flow dynamics in a liquid-solid fluidized bed at $(Re_p, \rho_r, Fr) = (25, 8, 0.51)$ and at three distinct times.

As suggested by different authors [36, 37], we define the height of the bed as the percentile 99 of the particles altitude (i.e. 99% of the particles are located below). Figure 4.12 shows the evolution of the bed height with time for the three cases investigated. As expected, the height of the bed and (therefore the porosity) increases with the superficial velocity. The oscillations around the mean value remain low after the start-up (less than one particle diameter), which confirms the homogeneous suspension regime. In the following, all time averages have been computed in the time interval $t^* \in [30, 120]$ when the bed is in pseudo steady-state.

The void fraction of the bed at a streamwise location z is computed by averaging the fluid phase indicator function χ_f in a cross section of the domain, i.e.

$$\phi_f(z) = \frac{1}{S} \int_{S(z)} \chi_f(\mathbf{x}) dS \quad (4.39)$$

As shown in Figure 4.13, the time average of the solid volume fraction $\bar{\phi}_s = 1 - \bar{\phi}_f$ reaches a constant value in the core of the bed, and this value decreases as the

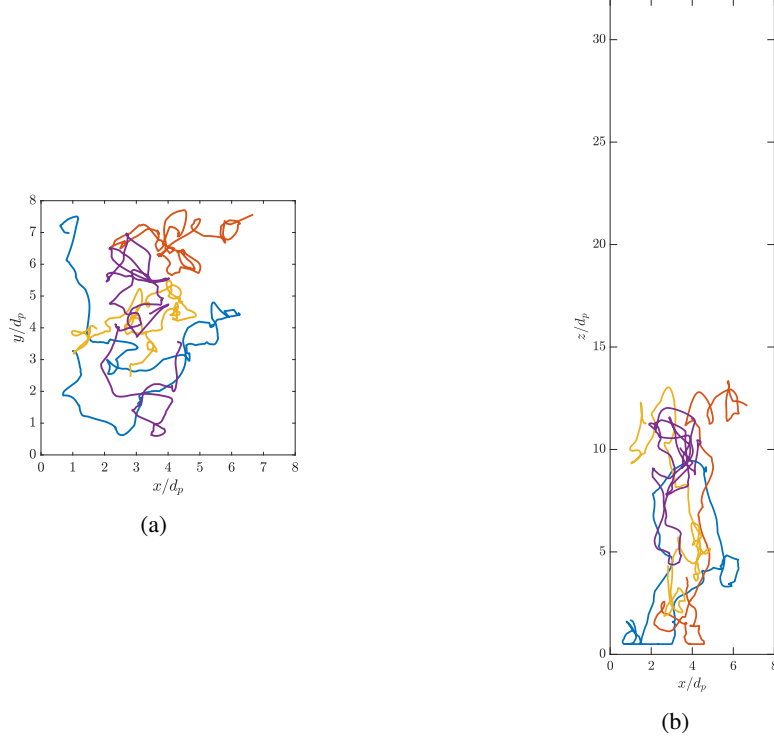


Figure 4.11: Projection of the trajectories of four particles in (a) a transverse xy plane and (b) a vertical xz plane at $Re_p = 25$.

superficial velocity increases. Then, the solid volume fraction decreases rapidly in the freeboard region at the top of the bed. As previously noted by Ozel et al. [95], the gradient of the solid volume fraction in the freeboard region becomes stiffer as the superficial velocity decreases. The spatial average of $\bar{\phi}_s$ between the streamwise positions $z_a = 2d_p$ and $z_b = 10d_p$ is used to estimate the mean porosity in the bed (reported in Table 4.2) as

$$\phi_{f,bed} = 1 - \frac{1}{(z_b - z_a)} \int_{z_a}^{z_b} \bar{\phi}_s(z) dz. \quad (4.40)$$

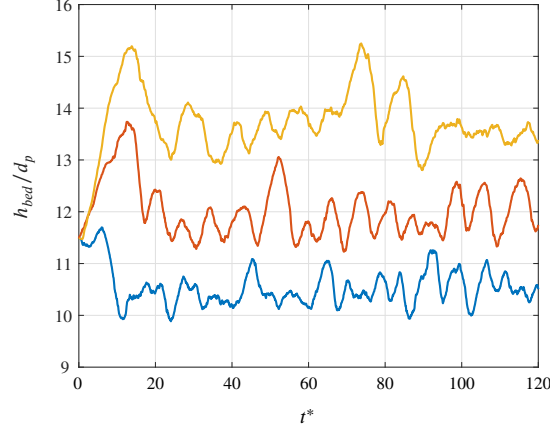


Figure 4.12: Time evolution of the bed height (99% definition) at $Re_p = 20$ (—), $Re_p = 25$ (—) and $Re_p = 30$ (—).

The streamwise extent of the region where the bed can be considered to be homogeneous and where we evaluate spatial averages is indicated by bounding boxes in Figure 4.13².

	$Re_p = 20$	$Re_p = 25$	$Re_p = 30$
$\phi_{f,bed}$	0.62	0.66	0.70

Table 4.2: Mean bed porosity.

Figure 4.14 confirms that the mean porosity of the bed is a linear function of the superficial velocity in a log-log diagram, in accordance with Richardson-Zaki's law (Eq. (4.23)). Yet, it must be acknowledged that the data were obtained over a limited range of bed void fractions. The slope of the linear regression on the three data points is $n = 2.90$, in fairly good agreement with the value $n = 2.80$ obtained from Eq. (4.24). There is however a vertical offset between our data and Richardson-Zaki's law if we assume $U_{0,\infty} = U_t$. This offset corresponds to the ratio between the value of the superficial velocity extrapolated at infinite dilution, $U_{0,\infty}$, and the estimation of the terminal velocity U_t , as discussed above. By extrapolating the linear regression to

²The choice of the bounds $z_a = 2d_p$ and $z_b = 10d_p$ was based on the case at $Re_p = 20$. Given the larger extent of the bed at $Re_p = 25$ and $Re_p = 30$, the right bound of the control volume could be slightly shifted towards the right for those two cases.

$\phi_{f,bed} = 1$, we obtain the ratio $k_u = \frac{U_{0,\infty}}{U_t} = 0.81$, in fairly good agreement with the value $k_u = 0.86$ obtained from the relation proposed by Rapagna et al. [103] outside the high voidage regime:

$$k_u = 1.09 - 0.11 \log_{10}(\text{Re}_t), \quad 50 < \text{Re}_t < 1000. \quad (4.41)$$

It must also be stressed that U_t has been estimated using Schiller-Naumann's drag law (Eq. (4.20)) and the iterative procedure described earlier, so that a fraction (that we assume small) of the offset is due to the error committed on the estimation of U_t .

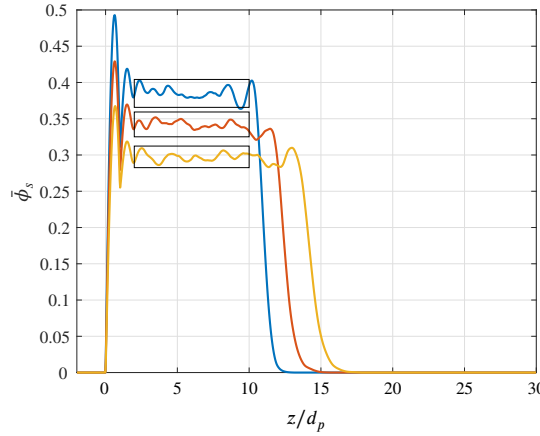


Figure 4.13: Time-averaged solid volume fraction profile at $\text{Re}_p = 20$ (—), $\text{Re}_p = 25$ (—) and $\text{Re}_p = 30$ (—).

As explained earlier, the pressure drop across the bed remains constant when the superficial velocity is increased beyond minimum fluidization. Our resolved simulations should be able to recover the correct pressure profile needed to compensate the weight of the bed. By integration of Eq. (4.2) in the vertical direction, we get

$$p(z) - p(z_{out}) = (\rho_s - \rho_f)g \int_z^{z_{out}} (1 - \phi_f(\tilde{z})) d\tilde{z}. \quad (4.42)$$

where the actual void fraction profile is used in the integral (i.e. not the mean value). We compare in Figure 4.15 the pressure profile predicted by Eq. (4.42) to the time-averaged pressure profile obtained from our resolved simulations. The latter is computed by taking the fluid-phase average of the pressure field in each cross section of the bed, i.e. $p_f(z) \triangleq \langle p \rangle_f(z)$. The pressure drop predicted by Eq. (4.42) is correctly

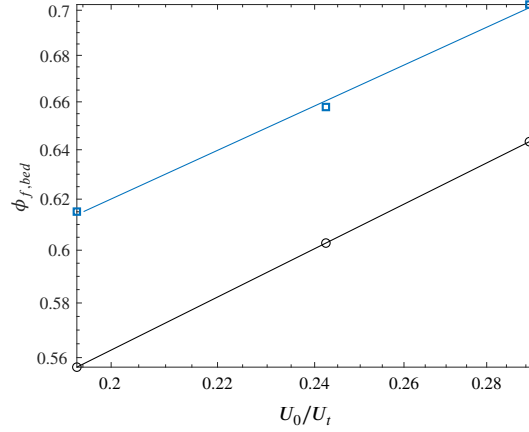


Figure 4.14: Mean porosity in the bed as a function of the superficial velocity ($\square$). Data are fitted to $\frac{U_0}{U_t} = k_u \phi_f^n$ with $k_u = 0.81$ and $n = 2.90$ (—). Richardson-Zaki's relation (Eq. (4.23)) with $k_u = 1$ and $n = 2.80$ is also shown ($\circ$).

reproduced by our simulations with a difference of only 1.2% for the most inertial case $Re_p = 30$. Note that, in order to visualize that the pressure drop remains constant as the superficial velocity increases, the pressure profiles have been normalized using the characteristic velocity U_c (see Eq. (4.35)) because it is a constant quantity in all three simulations, contrary to the superficial velocity U_0 .

The time average of the bed height using the 99% definition introduced above is reported in the first row of Table 4.3 for the three Reynolds numbers. Given that the volume of the bed $V_{bed} = h_{bed} S$ is related to the volume occupied by the solid phase through the bed porosity, the mean height of the bed can also be estimated from $\phi_{f,bed}$ as

$$h_{bed}^{(\phi_f)} = \frac{1}{S} \frac{N_p V_p}{(1 - \phi_{f,bed})}. \quad (4.43)$$

In addition, some authors [37, 135] proposed to estimate the bed height from the altitude where the total pressure corresponds to the hydrostatic pressure, or equivalently, where the dynamic pressure profile becomes zero (see Figure 4.15). It can be deduced from Table 4.3 that the two first methods produce almost identical results while using the pressure profile yields slightly lower values.

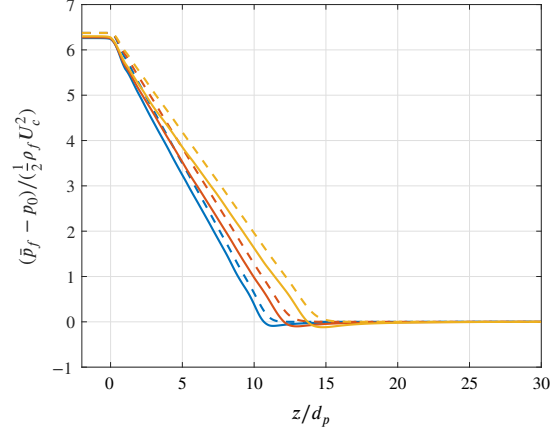


Figure 4.15: Time-averaged normalized pressure profile at $\text{Re}_p = 20$ (—), $\text{Re}_p = 25$ (—) and $\text{Re}_p = 30$ (—). The theoretical head losses given by Eq. (4.42) are also shown (---, --- and ---, respectively).

	$\text{Re}_p = 20$	$\text{Re}_p = 25$	$\text{Re}_p = 30$
$h_{bed}^{(99)}/d_p$	10.91	12.55	14.25
$h_{bed}^{(\phi_f)}/d_p$	10.94	12.51	14.21
$h_{bed}^{(p_f)}/d_p$	10.52	12.33	13.78

Table 4.3: Height of the fluidized bed estimated from the 99% definition, $h_{bed}^{(99)}$, the mean bed porosity, $h_{bed}^{(\phi_f)}$, and the time-averaged pressure profile, $h_{bed}^{(p_f)}$.

4.5.3 Particle velocity statistics

We now study in more details the statistics of particle motion in the bed. Figures 4.16a and 4.16b respectively show the time evolution of the vertical and transverse components of the mean particle velocity. As expected, they both oscillate around zero as there is no net flux of solids in the vertical and transverse directions. We can however observe that the oscillations in the vertical component are much stronger, for all Reynolds numbers. To evaluate the level of agitation in the bed, we present in Figures 4.16c and 4.16d the evolution of the standard deviation of the particle velocity in the vertical and transverse direction as a function of time. It can be observed that the level of the fluctuations is fairly insensitive to Re_p , but it is significantly larger in the

vertical direction. This observation is quantified by the anisotropy coefficient defined by Eq. (4.37) and whose values are reported in Table 4.4. Similarly to the settling problem that we addressed in the previous section, the anisotropy coefficient is constant in the range of bed porosities examined, viz. not the highly dilute regime. In addition, the values obtained from our simulations are consistent with those reported by previous studies [1, 95, 36], oscillating between 1.4 and 1.6 over a large range of Reynolds numbers.

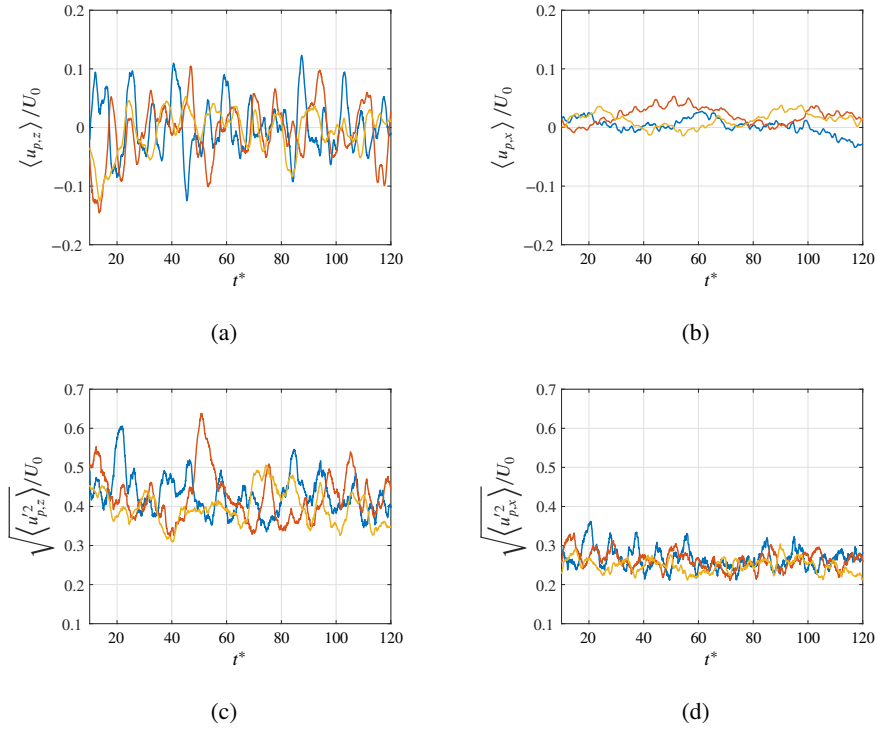


Figure 4.16: Time evolution of (a) the mean vertical component, (b) the mean transverse component, (c) the standard deviation of the vertical component and (d) the standard deviation of the transverse component of particle velocity in a liquid-solid fluidized bed at $Re_p = 20$ (—), $Re_p = 25$ (—) and $Re_p = 30$ (—).

	$Re_p = 20$	$Re_p = 25$	$Re_p = 30$
K_U	1.57	1.67	1.63

Table 4.4: Particle velocity anisotropy coefficient K_U .

Mean square displacement and self-diffusion coefficient

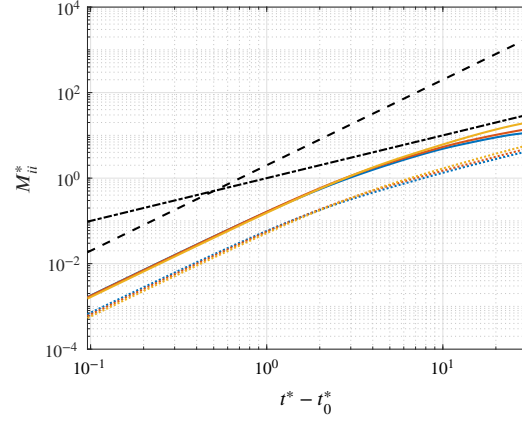
The dispersion motion of the particles in the bed can be characterized by the mean square displacement tensor,

$$M_{ij}(t) = \langle (x_{p,i}(t) - x_{p,i}(t_0))(x_{p,j}(t) - x_{p,j}(t_0)) \rangle, \quad (4.44)$$

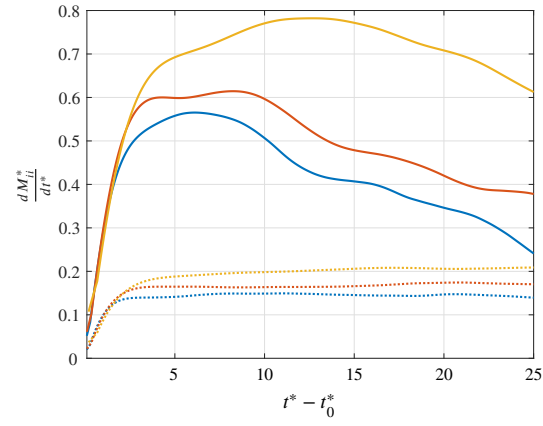
where $t - t_0$ is the time lag. When the motion of the particles is driven by diffusion, the diagonal components M_{ii} ($i = x, y$, or z) of the MSD tensor increase linearly with time, and the particle self-diffusion coefficient in direction i , defined as [1, 82, 99]

$$D_i = \frac{1}{2} \frac{dM_{ii}(t)}{dt}, \quad (4.45)$$

takes a constant value. This self-diffusive motion is the result of the small-scale hydrodynamic and collisional interactions that are decorrelated from the collective motions. We report in Figure 4.17a the evolution of the diagonal components of the MSD in the vertical and transverse directions in a log-log scale. The MSD in the transverse direction has been evaluated as $\frac{1}{2}(M_{xx} + M_{yy})$. To reduce statistical uncertainty, the MSD has been computed for different initial times t_0 after the startup transient period ($t_0^* > 30$). As reported in previous experimental [1], and numerical [36, 145, 37] studies, we observe in Figure 4.17a that the MSD deviates from a linear law at short times and fits instead a quadratic law, both in the transverse and vertical directions. This quadratic behavior is also expected theoretically [99, 82] as detailed in Appendix D. The linear growth of the MSD is observed at later times in the vertical and transverse directions. Yet, it can be observed that the MSD in the vertical dimension is flattening out for large separation times as a consequence of the limited bed height. Consequently, the time derivative of M_{zz} (Figure 4.17b) decreases after reaching a maximum. Hence, the existence of a diffusive motion in the vertical direction is limited in time due to the finite height of the bed. Conversely, the use of periodic boundary conditions in the transverse direction does not restrain the motion of the particles so that the MSD keeps increasing linearly with time and the self-diffusion coefficient maintains a constant value.



(a)



(b)

Figure 4.17: Time evolution of (a) the mean square displacement (log-log scale) and (b) the time derivative of the mean square displacement (linear scale) in the vertical (solid) and transverse (dotted) directions at $\text{Re}_p = 20$ (—, ···), $\text{Re}_p = 25$ (—, ···) and $\text{Re}_p = 30$ (—, ···). First (---) and second (- -) order power laws are shown in (a) for comparison.

Auto-correlation function

In order to determine the characteristic time and length scales of the agitation of the particles, it is interesting to examine the particle velocity auto-correlation function. Following the definition used in the works of Nicolai et al. [93] and others [36, 37], the auto-correlation function reads

$$R_{U_i U_i}(\tau) = \frac{\left\langle u'_{p,i}(t) u'_{p,i}(t + \tau) \right\rangle_t}{\left\langle u'^2_{p,i}(t) \right\rangle_t}, \quad (4.46)$$

where no summation is performed on the repeated index i and where τ is the separation time, or time lag. Figure 4.18 shows the auto-correlation functions for the three Reynolds numbers investigated in the vertical and transverse directions (global and close-up view close to the origin). In the transverse direction, the auto-correlation functions have been obtained as $\frac{1}{2} (R_{U_x U_x} + R_{U_y U_y})$ although we will simply refer to the x direction in what follows. For a purely Brownian motion, the auto-correlation function would decay exponentially towards zero [36]. The auto-correlation function in the vertical direction, $R_{U_z U_z}$, converges towards zero for long separation times but it first oscillates slightly around zero. This finding shows that particles exhibit a slight anti-correlated motion at intermediate time lags due to advective motions in the flow. The impact of the Reynolds number on the shape of the auto-correlation function is not clear in the vertical direction for large separation times. We suspect that our run times are a bit too short to reach complete time convergence. It can however be observed in the close-up view in Figure 4.18 that the decay of the auto-correlation function is slower as Re_p increases, which confirms previous findings of Ozel et al. [95] and Euzenat [37] who report longer correlation times as the superficial velocity, and therefore the bed height, increases. The auto-correlation function in the transverse direction converges faster and smoothly towards zero.

The particle velocity integral time scale in direction i is formally defined as

$$\mathcal{T}_{U_i} = \int_0^\infty R_{U_i U_i}(\tau) d\tau. \quad (4.47)$$

Given the lack of convergence of the auto-correlation function in the vertical direction for large time lags and the oscillatory motion induced by the large-scale structures, the particle velocity correlation time scale is estimated as the integral of the auto-correlation function from 0 to the first root τ_0 , which reads

$$\mathcal{T}_{U_i} \simeq \tau_{U_i} = \int_0^{\tau_0} R_{U_i U_i}(\tau) d\tau. \quad (4.48)$$

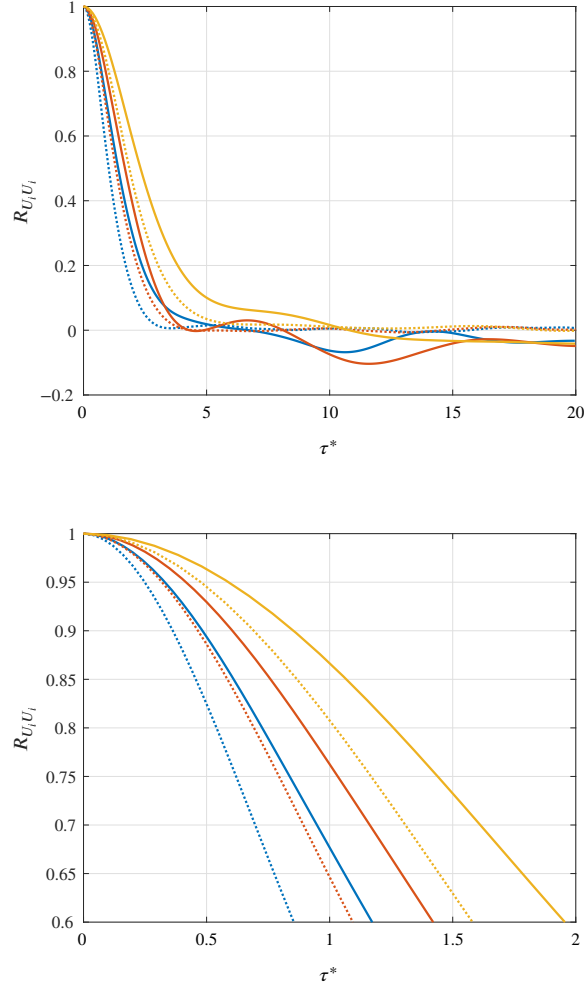


Figure 4.18: Global (top) and close-up view (bottom) of the particle velocity auto-correlation function in the vertical (solid) and transverse (dotted) directions at $Re_p = 20$ (—, ···), $Re_p = 25$ (—, ···) and $Re_p = 30$ (—, ···).

The fluctuation length scale can then be approximated by using the correlation time scale and the standard deviation of the particle velocity:

$$l_{U_i} = \sqrt{\langle u_{p,i}^2 \rangle_t} \tau_{U_i}. \quad (4.49)$$

We report in Table 4.5 the particle velocity correlation time and length scales in the transverse and vertical directions. As previously inferred from Figure 4.18, the correlation time scale is larger in the vertical direction owing to the influence of the mean flow, and it globally increases with the Reynolds number. Esteghamatian et al. [36] report slightly lower values for the correlation length scales ($l_{U_x}^* = 0.160$ and $l_{U_z}^* = 0.326$) but at significantly lower Reynolds number ($Re_p = 6$) and lower porosity ($\phi_{f,bed} = 0.54$).

	$Re_p = 20$	$Re_p = 25$	$Re_p = 30$
$\tau_{U_x}^*$	1.17	1.48	2.23
$\tau_{U_z}^*$	1.63	1.78	2.80
$l_{U_x}^*$	0.32	0.38	0.54
$l_{U_z}^*$	0.70	0.76	1.11

Table 4.5: Particle velocity correlation time and length scales in the transverse (x) and vertical (z) directions in liquid-solid fluidized beds.

As detailed in Appendix D, the self-diffusion coefficient defined by Eq. (4.45) can be related to the particle velocity correlation time scale as

$$D_i = \left\langle u_{p,i}^2 \right\rangle_t \tau_{U_i} \simeq \left\langle u_{p,i}^2 \right\rangle_t \tau_{U_i} = l_{U_i}^2 / \tau_{U_i}, \quad (4.50)$$

with no summation on the repeated index i . Hence, we have two ways of computing the self-diffusion coefficient: either from the slope of the mean square displacement when the latter evolves linearly with time, or using the correlation time and length scales derived from the autocorrelation function (ACF). The values obtained from the two methods are compared in Table 4.6. In the vertical direction, the value of the self-diffusion coefficient has been evaluated from the MSD using the maximum value of its time derivative in Figure 4.17b, before the effect of the limited bed height is visible. In the transverse direction, the diffusion coefficient has been evaluated from the constant value reached by the time derivative of the MSD. The comparison between the two approaches shows a good agreement, although the auto-correlation function returns systematically larger values both in the transverse and vertical directions. The discrepancy can be partly explained by the lack of time convergence and the approximate definition of the particle velocity correlation time scale (see Eq. (4.48)), as well as by the imperfect evaluation of the vertical diffusion coefficient from the MSD. In any case, these results show that the self-diffusion coefficient in the vertical direction is 3 to 4 times larger than in the transverse direction.

		$Re_p = 20$	$Re_p = 25$	$Re_p = 30$
$\mathcal{D}_x^*$	MSD	0.068	0.084	0.10
	ACF	0.086	0.097	0.13
$\mathcal{D}_z^*$	MSD	0.28	0.31	0.39
	ACF	0.30	0.32	0.44

Table 4.6: Particle self-diffusion coefficient in the transverse (x) and vertical (z) directions evaluated from the mean square displacement (MSD) and from the auto-correlation function (ACR).

4.5.4 Force statistics

Mean fluid-particle force

We first examine the mean value of the force exerted by the fluid on a particle in the bed. Figure 4.19 shows the evolution of the mean vertical component of the fluid-particle force as a function of the Reynolds number. The force has been scaled by the Stokes drag,

$$F_{St} = 3\pi\mu d_p U_0. \quad (4.51)$$

The comparison with literature correlations derived from DNS studies on static particle arrays is very satisfactory. It must also be stressed that in the case of fluidized beds, the Reynolds number Re_p and the void fraction ϕ_f are interdependent, so that Figure 4.19 does not represent the evolution of the fluid-particle force at fixed porosity. Several authors [124, 68] reported an increase of the dimensionless drag force in gas-solid suspensions with respect to the static case, but this effect is not clearly identified in our results for liquid-solid fluidized beds. This point is discussed in more details in Section 4.6.

Fluid-particle force distribution

We now investigate the distribution of the fluid-particle force in these liquid-solid fluidized beds. We show in Figure 4.20 the pdf's of the vertical and transverse components of the force for the particles located in the region of the bed bounded by $z_a = 2d_p$ and $z_b = 10d_p$ (see bounding boxes in Figure 4.13), and for all sampled times after $t^* > 30$. The force has been here scaled by the buoyancy force,

$$F_b = V_p(\rho_s - \rho_f)g. \quad (4.52)$$

It must be mentioned that the distributions have been "truncated" horizontally between 0 and 2 for the vertical component and between -1 and 1 for the transverse component.

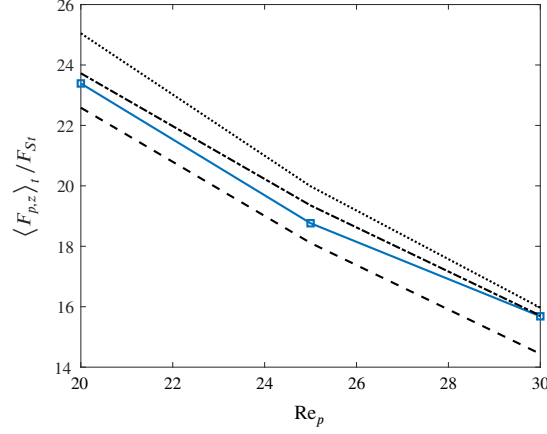


Figure 4.19: Mean vertical component of the fluid-particle force as a function of the Reynolds number ($\square$). Comparison with drag correlations of Tenneti et al [134] (—), Beetstra et al. [9] (---) and Tang et al. [124] (····).

Most of the data are covered in those intervals: the area under the truncated pdf's of $F_{p,z}$ and $F_{p,x}$ represent respectively 98.2% and 98.4% of the total area. However, it is later shown that the complete (i.e. non-truncated) distributions of the components of the force display a "heavy-tailed" behavior for very large values. In a first step, we characterize these distributions in their main part.

We report in Table 4.7 the main statistics (i.e. the first moments) of the vertical and transverse components of the force, evaluated from the truncated distributions. The standard deviation of the i th component of the force is defined as

$$\sigma_{F_{p,i}} = \sqrt{\langle F_{p,i}'^2 \rangle_t}. \quad (4.53)$$

The skewness and kurtosis are respectively defined as

$$S_{F_{p,i}} = \frac{\langle F_{p,i}'^3 \rangle_t}{\sigma_{F_{p,i}}^3} \quad (4.54)$$

and

$$\mathcal{K}_{F_{p,i}} = \frac{\langle F_{p,i}'^4 \rangle_t}{\sigma_{F_{p,i}}^4}. \quad (4.55)$$

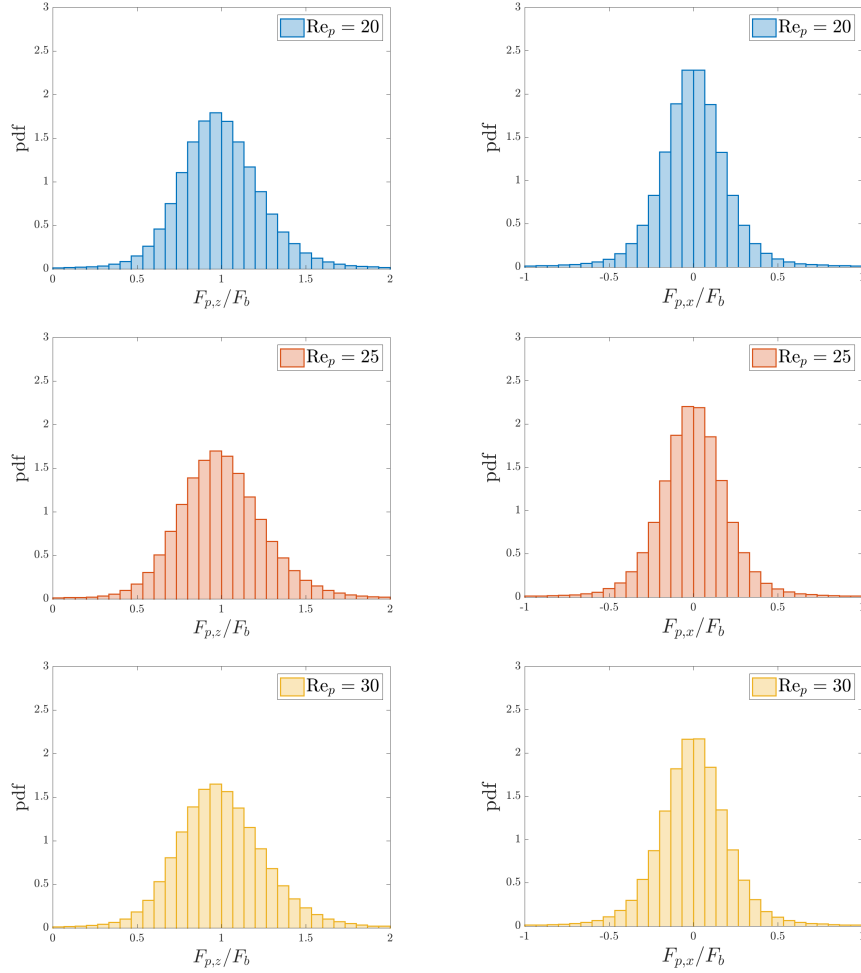


Figure 4.20: Distribution of the vertical (left) and transverse (right) components of the fluid-particle force in the core region of liquid-solid fluidized beds (control volume bounded by $z_a = 2d_p$ and $z_b = 10d_p$).

First, the data confirm that the mean value of the vertical component of the force compensates correctly the buoyancy force F_b , by definition of the fluidized state. The standard deviation of the vertical component of the force is larger than that of the transverse component, and it is also seen that $\sigma_{F_{p,z}}$ increases slightly with Re_p . In Chapter 2, we found that $\sigma_{F_{p,z}}$ increases with the Reynolds number and with the porosity of the bed. In

the case of a fluidized bed, the two factors are coupled, but the range of regimes that we investigated here is quite limited so that the increase of $\sigma_{F_{p,z}}$ in Table 4.7 is fairly small. The distribution of $F_{p,z}$ is slightly right-skewed (positive skewness). This feature was also observed in fixed particle arrays in Chapter 2. Conversely, the distribution of $F_{p,x}$ is perfectly symmetric (zero skewness). The kurtosis of both distributions is above 3 (the theoretical value for a normal distribution), and this effect is more pronounced for the transverse component of the force.

Re_p	$\frac{\langle F_{p,z} \rangle_t}{F_b}$	$\frac{\sigma_{F_{p,z}}}{\langle F_{p,z} \rangle_t}$	$S_{F_{p,z}}$	$\mathcal{K}_{F_{p,z}}$	$\frac{\langle F_{p,x} \rangle_t}{F_b}$	$\frac{\sigma_{F_{p,x}}}{\langle F_{p,x} \rangle_t}$	$S_{F_{p,x}}$	$\mathcal{K}_{F_{p,x}}$
20	0.996	0.249	0.23	4.0	-3.0×10^{-4}	0.209	7.8×10^{-3}	5.4
25	1.001	0.257	0.24	3.8	-1.0×10^{-4}	0.209	2.5×10^{-3}	5.1
30	0.999	0.263	0.22	3.7	7.7×10^{-5}	0.215	2.2×10^{-3}	5.0

Table 4.7: Statistics of the fluid-particle force in liquid-solid fluidized beds (truncated distributions).

It is also worthwhile to compare the characteristics of the distribution of the fluid-particle force in homogeneous fluidized beds with the results obtained for fixed random arrays of particles. We consider here the case of the liquid-solid fluidized bed at $\text{Re}_p = 30$. The time-averaged porosity in the bed is $\phi_{f,bed} = 0.70$ (see Table 4.2). To make the comparison, and similarly to what was done in Chapter 2, we computed the flow past randomly distributed arrays of particles for the set of parameters $(\text{Re}_p, \phi_s) = (30, 0.30)$. Data have been collected over three independent realizations of the flow. Figure 4.21 compares the distributions of the vertical and transverse components of the force in the fixed and fluidized cases and we report their main statistics in Table 4.8. For the fluidized bed, the statistics are still evaluated using the truncated distributions. First,

	$\frac{\langle F_{p,z} \rangle_t}{F_{St}}$	$\frac{\sigma_{F_{p,z}}}{\langle F_{p,z} \rangle_t}$	$\frac{\sigma_{F_{p,x}}}{\langle F_{p,x} \rangle_t}$
Fixed bed	15.59	0.268	0.172
Fluidized bed	15.88	0.262	0.214

Table 4.8: Comparison of the fluid-particle force statistics in a fixed bed and in a liquid-solid fluidized bed at $(\text{Re}_p, \phi_s) = (30, 0.30)$.

the data confirm that, in this regime, the mean fluid-particle force is not significantly modified by the agitation of the particles. Furthermore, it appears that the standard deviation of $F_{p,z}$ is similar in both cases, which is confirmed by the similar shape of the

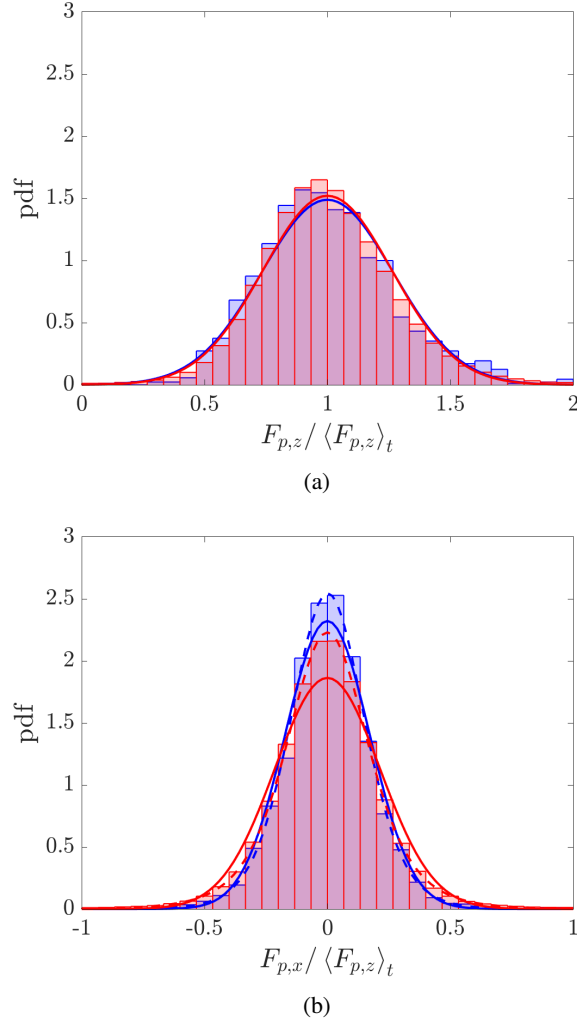


Figure 4.21: Distribution of the (a) vertical and (b) transverse components of the fluid-particle force in a fixed bed (blue) and in a liquid-solid fluidized bed (red) at $(Re_p, \phi_s) = (30, 0.30)$. Data are fitted to a normal distribution (—, —) in (a) and (b) and to a location-scale t-distribution (- - , - -) in (b).

two pdf's in Figure 4.21a. A normal distribution (solid line) fits reasonably well the pdf in both cases, despite the slight skewness of the distribution. In the transverse direction, the standard deviation of the force increases slightly as we move from the fixed to the

fluidized bed case. This can also be observed on the distribution of $F_{p,x}$ in Figure 4.21b. Both in the fixed bed and the fluidized bed cases, the fitted normal distribution underestimates the peak of the pdf, and this effect is even more pronounced for the fluidized bed. In comparison, it is seen that a location-scale t-distribution (dashed line) matches the data more accurately. The pdf of a location-scale t-distribution is defined as

$$f(x|\mu, \sigma, \nu) = \frac{1}{\sigma\sqrt{\pi\nu}} \frac{\Gamma\left(\frac{\nu+1}{2}\right)}{\Gamma\left(\frac{\nu}{2}\right)} \left(\frac{\nu + \left(\frac{x-\mu}{\sigma}\right)^2}{\nu} \right)^{-\left(\frac{\nu+1}{2}\right)}, \quad (4.56)$$

so that $\frac{x-\mu}{\sigma}$ follows a standard Student's t-distribution, with a zero mean and a variance equal to $\frac{\nu}{\nu-2}$. In the present case, $x = \frac{F_{p,x}}{\langle F_{p,z} \rangle_t}$. When $\nu \rightarrow \infty$, Eq. (4.56) corresponds to the pdf of a standard normal distribution. Since the distributions in Figure 4.21b are obviously centered around zero ($\mu = 0$), we only discuss the scaling parameter σ and the number of degrees of freedom ν . In the fixed bed case, the parameters of the fitted t-distribution are $(\sigma, \nu) = (0.15 \pm 7.1 \times 10^{-3}, 9.4 \pm 2.7)$. The number of degrees of freedom ν is quite large and the difference with a normal distribution is thus moderate. In the fluidized bed case, the parameters of the fitted t-distribution are $(\sigma, \nu) = (0.17 \pm 5.0 \times 10^{-4}, 5.3 \pm 6.7 \times 10^{-2})$. The number of degrees of freedom is significantly smaller (as well as the confidence interval), which confirms the stronger deviation from a normal distribution.

We now consider the complete (i.e. non-truncated) distribution of the fluid-particle force in the liquid-solid fluidized bed at $Re_p = 30$. More specifically, we focus on its behavior for values located far from the average. Figure 4.22b shows that the distribution of $F_{p,z}$ is "heavy tailed", in the sense that it decreases much more slowly than the normal distribution fitted on its main part. The right tail of the pdf of $x = \frac{(F_{p,z} - \langle F_{p,z} \rangle_t)}{\langle F_{p,z} \rangle_t}$ is plotted in a log-log diagram in Figure 4.22a. It can be concluded that the right tail of the pdf is governed by a power law distribution of the type $y = Cx^{-p}$, with $p = 2.41$. The black curve in Figure 4.22b confirms that this power law distribution nicely represents the evolution of the pdf for very large values of the force. Because the exponent p of this power law is between 2 and 3, the first moment of the distribution is well defined, but the second moment (i.e. the variance) diverges. Indeed, we have that

$$\int_a^\infty \frac{x^2}{x^p} dx \rightarrow \infty, \quad \forall a \geq 0, \quad \forall p \leq 3. \quad (4.57)$$

This result implies that the accumulation of data will not allow the variance (and standard deviation) of the force to converge. This also justifies that we have previously truncated the distributions to make a comparison with the fixed bed case. The same findings are made for the left tail of the distribution in Figure 4.23, but with an even smaller exponent, $p = 2.17$. This difference is attributable to the slight skewness of the distribution.

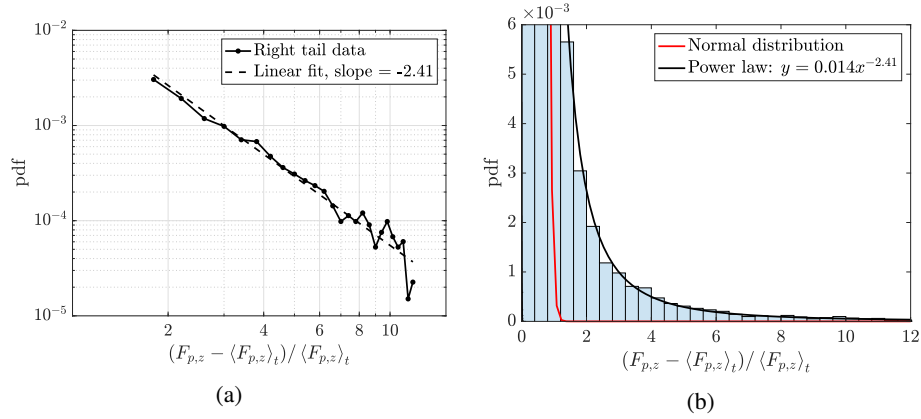


Figure 4.22: Right tail of the distribution of the vertical component of the fluid-particle force in the liquid-solid fluidized bed at $Re_p = 30$ in (a) log-log scale and (b) linear scale.

Finally, we also examine the transverse component of the force, see Figure 4.24. The normal distribution and the t-distribution that were fitted on the main part have a much faster decay than the true distribution. In this case, the exponent of the power law is $p = 2.26$ and the behavior of the tail is left-right symmetric.

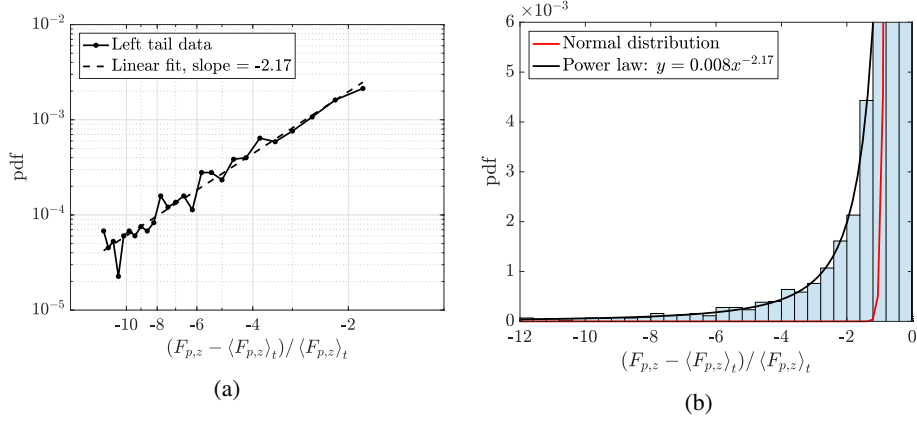


Figure 4.23: Left tail of the distribution of the vertical component of the fluid-particle force in the liquid-solid fluidized bed at $Re_p = 30$ in (a) log-log scale and (b) linear scale.

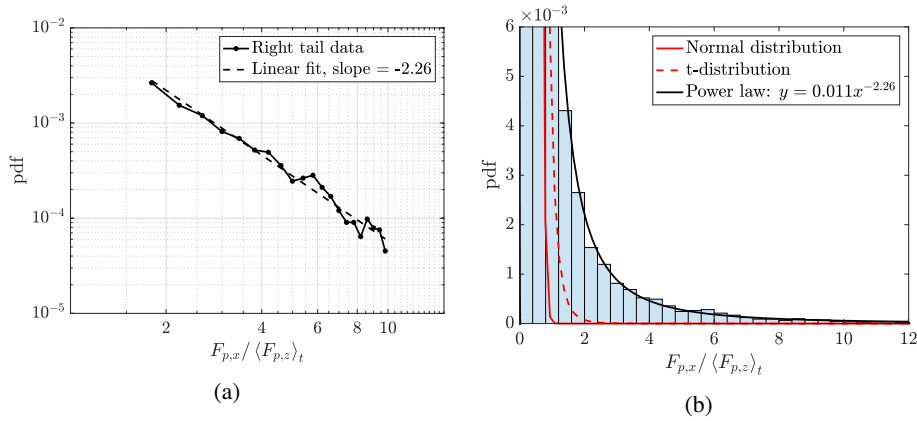


Figure 4.24: Right tail of the distribution of the transverse component of the fluid-particle force in the liquid-solid fluidized bed at $Re_p = 30$ in (a) log-log scale and (b) linear scale. The left tail is similar as there is no skewness.

Auto-correlation function

The auto-correlation function of the i th component of the fluid-particle force is defined similarly to Eq. (4.46) as

$$R_{F_i F_i}(\tau) = \frac{\left\langle F'_{p,i}(t) F'_{p,i}(t + \tau) \right\rangle_t}{\left\langle F'_{p,i}(t) F'_{p,i}(t) \right\rangle_t}. \quad (4.58)$$

As shown in Figure (4.58), both $R_{F_x F_x}$ and $R_{F_z F_z}$ decrease to a minimum negative value and then oscillate slightly before converging towards zero. The decrease is slower as the Reynolds number increases. Similar to the particle velocity, the fluid-particle force integral time scale reads

$$\mathcal{T}_{F_i} = \int_0^\infty R_{F_i F_i}(\tau) d\tau. \quad (4.59)$$

Its approximation using the first root τ_0 of the auto-correlation function is given by

$$\tau_{F_i} = \int_0^{\tau_0} R_{F_i F_i}(\tau) d\tau. \quad (4.60)$$

The auto-correlation function of the fluid-particle force looks more converged than that of the particle velocity and shows less oscillations at large separation times. Hence, we compare in Table 4.9 the values obtained using the exact definition of the integral time scale (Eq. (4.59)) and the approximation given by Eq. (4.60). As expected from the shape of the auto-correlation functions, the values of $\tau_{F_i}^*$ are always larger than those of $\mathcal{T}_{F_i}^*$. Similarly to what was observed for the particle velocity, the correlation time of the fluid-particle force is larger in the vertical than in the transverse direction and increases with the Reynolds number. We report in Figure 4.26 the values of $\mathcal{T}_{F_z}^*$ given in Table 4.9 and those reported by Esteghamatian et al. [35] from their resolved simulations of low Reynolds number liquid-solid fluidized beds. Quite interestingly, the simple linear fit

$$\mathcal{T}_{F_z}^* = 0.354 + 0.0211 \text{Re}_p \quad (4.61)$$

reproduces fairly well the evolution of $\mathcal{T}_{F_z}^*$ over the whole range of Reynolds numbers.

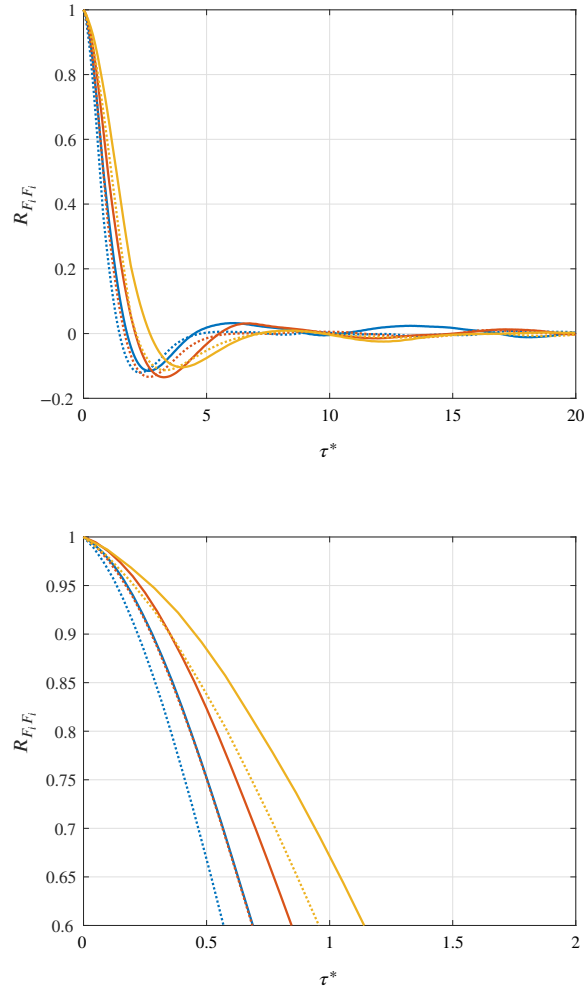


Figure 4.25: Global (top) and close-up view (bottom) of the fluid-particle force auto-correlation function in the vertical (solid) and transverse (dotted) directions at $Re_p = 20$ (—, ···), $Re_p = 25$ (—, ···) and $Re_p = 30$ (—, ···).

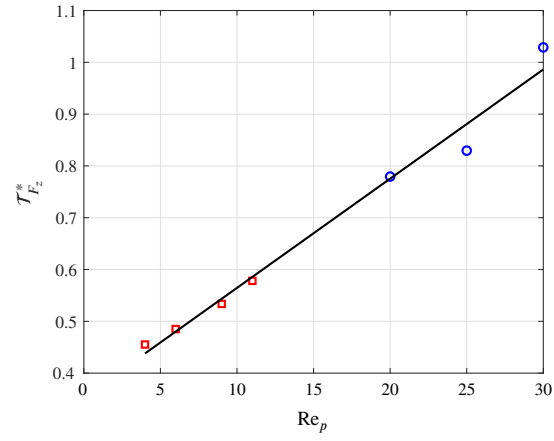


Figure 4.26: Integral time scale of the vertical fluid-particle force component as a function of the Reynolds number. PR-DNS data of Esteghamatian et al. [35] ($\square$) and ours ($\circ$) are fitted to a linear model (—).

	$\text{Re}_p = 20$	$\text{Re}_p = 25$	$\text{Re}_p = 30$
$\mathcal{T}_{F_x}^*$	0.51	0.55	0.77
$\mathcal{T}_{F_z}^*$	0.78	0.84	1.03
$\tau_{F_x}^*$	0.70	0.82	1.11
$\tau_{F_z}^*$	0.85	1.04	1.34

Table 4.9: Fluid-particle force correlation time scales in the transverse (x) and vertical (z) directions.

4.5.5 Heat transfer

We now examine the thermal problem in liquid-solid fluidized beds. As mentioned earlier, the resolved simulation of the heat transfer between the liquid and the solid particles is numerically challenging due to the fairly high Prandtl number ($Pr = 7$) and the resulting thin boundary layer. The fluid enters the domain at a temperature T_0 while the solid particles have a fixed temperature T_s . The instantaneous temperature field is shown in Figure 4.27 for the three Reynolds numbers.

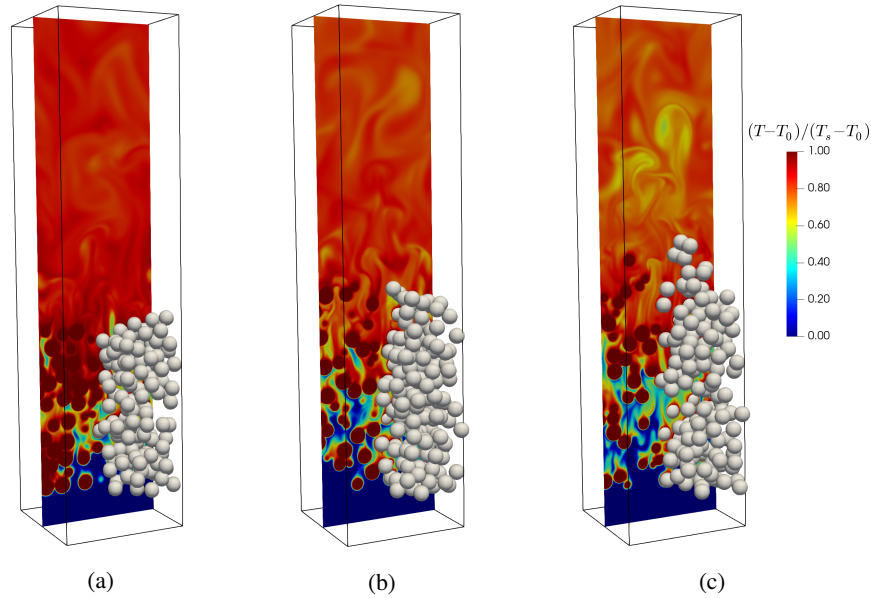


Figure 4.27: Instantaneous temperature field in a liquid-solid fluidized bed at (a) $Re_p = 20$, (b) $Re_p = 25$, c) $Re_p = 30$.

As a reminder, the bulk temperature at a local streamwise position z is defined as

$$T_b(z) = \frac{\int_{S_f(z)} u_z T \, dS}{\int_{S_f(z)} u_z \, dS}. \quad (4.62)$$

The time-averaged bulk temperature profiles shown in Figure 4.28 indicate that the fluid reaches higher temperatures as the Reynolds number decreases. These observations corroborate our earlier discussion in Chapter 3, where it was shown that dense

and viscous regimes lead to faster thermal saturation. The black dotted lines in Figure 4.28 indicate the control volume bounded by the streamwise positions $z_a = 2d_p$ and $z_b = 10d_p$ where averages will be evaluated, thus avoiding the thermal entrance region and the outlet of the bed. To evaluate the heat flux $Q_{s \rightarrow f}$ exchanged between the

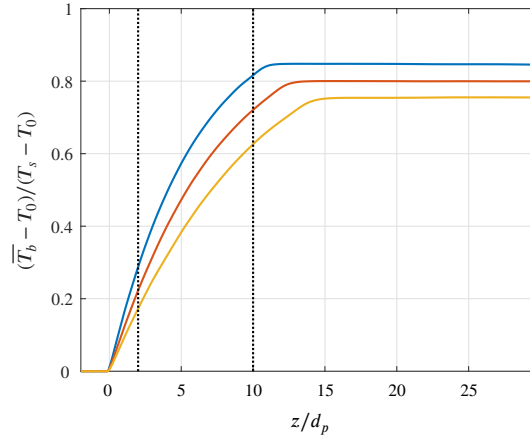


Figure 4.28: Time-averaged bulk temperature profile at (a) $Re_p = 20$ (—), (b) $Re_p = 25$ (—), (c) $Re_p = 30$ (—).

fluid and the solid phases, we perform a heat balance in the fluid phase as detailed in Chapter 3:

$$Q_{s \rightarrow f} = \left(\int_{S_b} \chi_f \rho_f c_{p,f} u_z T \, dS - \int_{S_b} \chi_f k_f \frac{\partial T}{\partial z} \, dS \right) - \left(\int_{S_a} \chi_f \rho_f c_{p,f} u_z T \, dS - \int_{S_a} \chi_f k_f \frac{\partial T}{\partial z} \, dS \right), \quad (4.63)$$

where S_a and S_b correspond to the domain cross sections at $z = z_a$ and $z = z_b$, respectively. The volumetric interphase heat flux is then obtained as

$$q_{s \rightarrow f} = \frac{Q_{s \rightarrow f}}{V}, \quad (4.64)$$

where $V = (z_b - z_a)S$. Then, an instantaneous Nusselt number based on the bulk temperature can be defined as

$$Nu_b(t) = \frac{q_{s \rightarrow f}(t) d_p^2}{6 \phi_s(t) k_f (T_s - T_{b,m}(t))} \quad (4.65)$$

where $T_{b,m}$ is the mean bulk temperature in the control volume,

$$T_{b,m}(t) = \frac{1}{(z_b - z_a)} \int_{z_a}^{z_b} T_b(z, t) dz. \quad (4.66)$$

and $\phi_s(t)$ corresponds to the (instantaneous) spatial average of the solid volume fraction in the control volume. Figure 4.29 shows the evolution of the Nusselt number in the control volume as a function of time. The time averages of the Nusselt number (indicated by dashed lines in Figure 4.29) are reported in Figure 4.30 as a function of the Reynolds number and compared to the correlations of Gunn [53], Deen et al. [25] and Sun et al. [120]. Again, it must be stressed that since the Reynolds number and the bed porosity are interdependent in fluidized beds, Figure 4.30 does not reproduce the dependence of the Nusselt number on the Reynolds number at fixed void fraction. In the regimes investigated, literature correlations predict constant or very slightly decreasing values for the Nusselt number with Gunn's relation [53] predicting much higher values, as noted in Chapter 3. The estimations of the Nusselt number from our simulations are somewhat higher than those predicted by Deen et al. [25] and they appear to increase with the Reynolds number. It is unclear whether this effect is caused by the finite resolution of the grid (and the resulting overestimation of the heat flux) or whether it reveals an enhancement of the heat transfer with particle agitation.

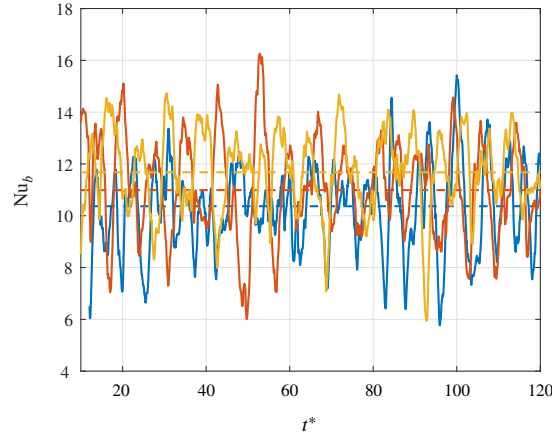


Figure 4.29: Time evolution of the Nusselt number at (a) $Re_p = 20$ (—), (b) $Re_p = 25$ (—), (c) $Re_p = 30$ (—). Dashed lines indicate the corresponding time-averaged values.

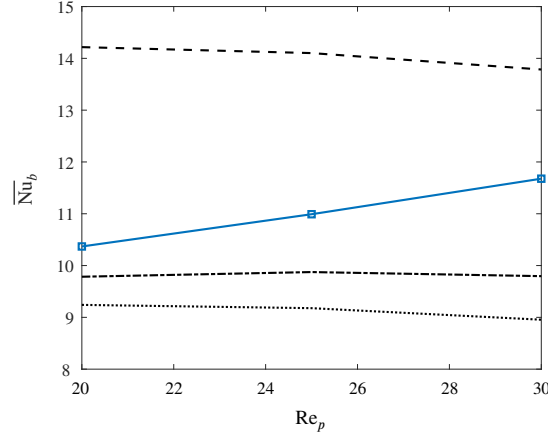


Figure 4.30: Time-averaged Nusselt number as a function of the Reynolds number (—■—). Comparison with the correlations of Gunn [53] (---), Deen et al. [25] (-·-) and Sun et al. [120] (···).

We show in Figure 4.31 the distribution of the normalized heat flux Q_p^* and the particle Nusselt number $Nu_b^{(p)}$, respectively defined as

$$Q_p^* = \frac{Q_p d_p}{S_p k_f (T_s - T_{b,m})} \quad (4.67)$$

and

$$Nu_b^{(p)} = \frac{Q_p d_p}{S_p k_f (T_s - T_b(z_p))} \quad (4.68)$$

The values reported in the histogram have been obtained for all times after $t^* = 30$ and inside the control volume bounded by $z_a = 2d_p$ and $z_b = 10d_p$. Due to thermal saturation, the normalized heat flux distribution shows a skewed shape as already observed in fixed beds in Chapter 3, and the skewness increases in dense regimes (i.e. at low Re_p in the present case). The normalization of the heat flux by the local bulk temperature $T_b(z_p)$ (evaluated at the streamwise position of the particle) in the definition of $Nu_b^{(p)}$ allows to reduce only marginally the skewness of the distribution and the occurrence of near-zero values. In addition, the mean values of Q_p^* and $Nu_b^{(p)}$ are compared to the time-averaged Nusselt number $\overline{Nu}_b$ obtained from a heat balance in the fluid phase (Eq. (4.65)). Although they should give similar results, we can observe that the evaluation of the mean interfacial heat flux from a Lagrangian perspective produces larger

values, and the difference with the mean Nusselt number evaluated from the fluid phase increases in dense regimes. Similar conclusions were drawn in Chapter 3, although the deviation seems more significant here. The mean Nusselt number calculated from the heat balance on the fluid phase is more reliable as it does not depend on the accuracy of the pdf reconstruction and is not affected by possible outlier effects. The discrepancy between the two approaches should however be more deeply investigated.

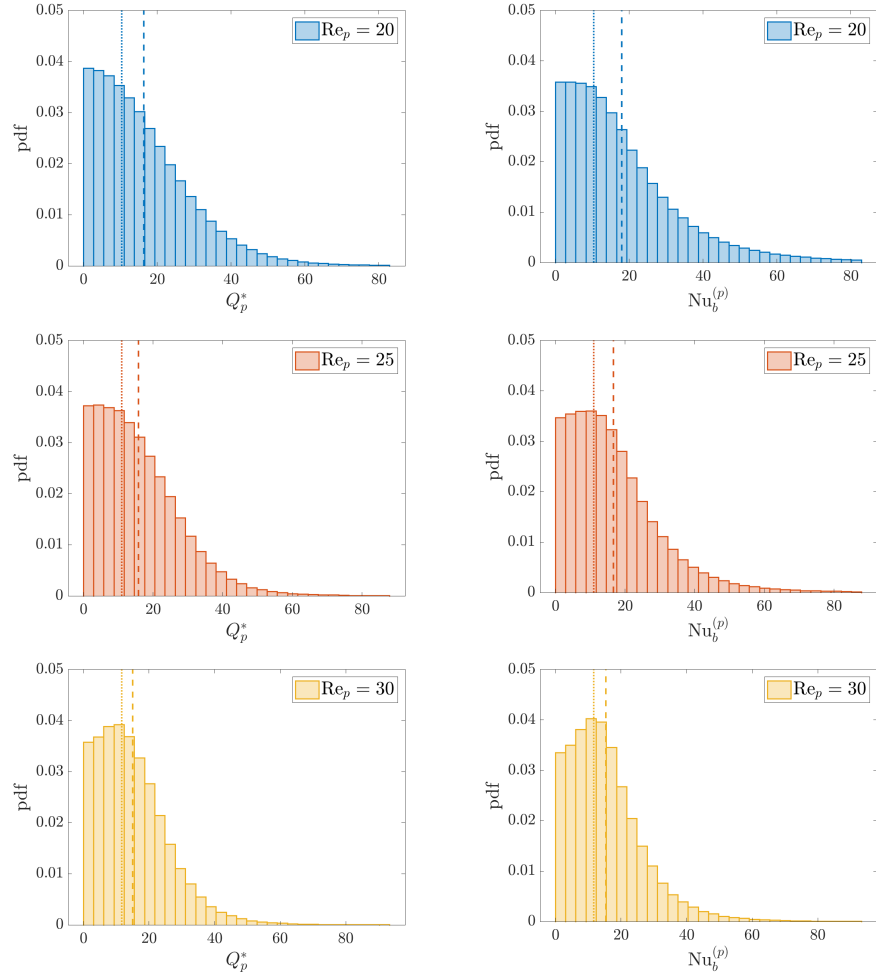


Figure 4.31: Distribution of the normalized heat flux (left) and the particle Nusselt number (right) for the different Reynolds numbers. Vertical dashed lines indicate the mean value of the distribution while dotted lines correspond to $\overline{Nu}_b$, the time average of the Nusselt number evaluated from the fluid-phase heat balance (Eq. (4.65)).

4.6 Gas-solid fluidized beds

The liquid-solid fluidized beds studied in the previous section correspond to homogeneous suspensions in a wide range of physical and operating parameters. Conversely, gas-solid fluidized beds exhibit a much more heterogeneous behavior, involving the formation of large voids, or bubbles, and the clustering of particles. Those phenomena are related to the significantly larger inertia of the solid particles in a gas, compared to a liquid. The Stokes number (see Eq. (4.38)) of gas-solid fluidized beds is typically in the range $\mathcal{O}(100)$ to $\mathcal{O}(1000)$. In the following, we study through resolved simulations the dynamics of gas-solid fluidized beds and we highlight the main differences with respect to the liquid-solid fluidization regime. In addition we discuss the impact of two parameters: the size of the transverse dimensions and the type of boundary conditions (periodic or solid walls).

4.6.1 Numerical set-up

We performed resolved simulations of bi-periodic gas-solid fluidized beds using $N_p = 1024$ (case 1) and $N_p = 2304$ (case 2A) solid particles. As for liquid-solid fluidized beds, the inflow is located at $z = -2d_p$ and a virtual grid is placed at $z = 0$. As shown in Figure 4.32, the two domains have the same vertical dimension $L_z = 64d_p$, but the transverse dimension is increased from $L_x = L_y = 8d_p$ in the first case to $12d_p$ in the second case. Hence, the two systems correspond to the same packed bed height. Indeed, the 1024 particles can be stacked in a regular array of $8 \times 8 \times 16$ spheres while the 2304 particles can be stacked in a $12 \times 12 \times 16$ array. The solid-fluid density ratio is $\rho_r = 1000$, which gives a Stokes number $St = 166.7$. Other physical and numerical parameters are given in Table 4.10. For the case containing 2304 particles, we also investigate the influence of the transverse boundary conditions by performing a resolved simulation using solid walls in the x and y directions (case 2B). The same collision parameters (e_n, e_t, μ_c) have been used for particle-particle and particle-wall contacts. Hence, in case 2B, particles undergo unelastic collisions with the side walls. The case 1 ran for 9 days on 512 processors (~ 110000 cpu.hours) while cases 2A and 2B ran for 10 days on 2048 processors (~ 490000 cpu.hours each).

4.6.2 Flow visualization, bed height and pressure drop

Figure 4.33 shows the evolution of the bi-periodic gas-solid fluidized bed with $N_p = 1024$ particles at three successive times. We can observe that the bed is far from being homogeneous, with the emergence and growth of a slug (i.e. a large region free of par-

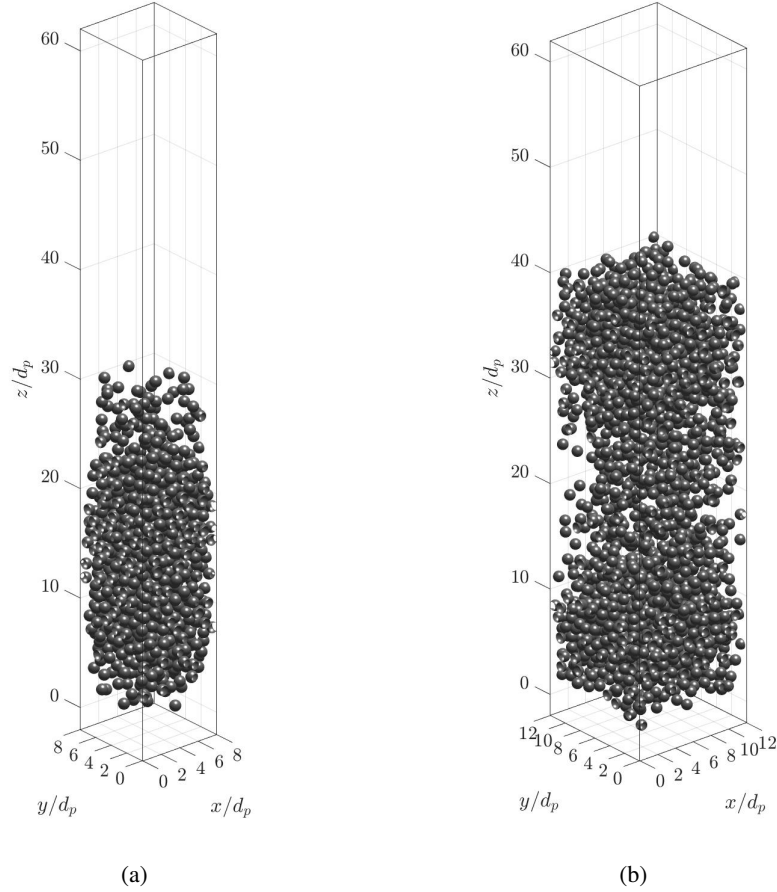


Figure 4.32: Computational domain and initial configuration of (a) 1024 and (b) 2304 particles for the resolved simulation of gas-solid fluidized beds.

ticles) that rises vertically and pushes the bed in a piston-like fashion. At some point, the slug bursts and the solid particles trickle down the bed. This episodic motion is maintained by the voids that are created at the entrance of the bed and merge into a single slug. Due to the limited transverse dimensions, the slug takes the entire width of the bed. By comparison, Figure 4.34 shows the dynamics of the case with $N_p = 2304$ particles in the wider domain and also with periodic conditions (case 2A). The growth and rise of a gas bubble is still visible but it does not cause a full break up of the bed.

Fluid density	ρ_f	1	[kg/m ³]
Solids density	ρ_s	1000	[kg/m ³]
Fluid kinematic viscosity	ν	2×10^{-5}	[m ² /s]
Gravitational acceleration	g	9.81	[m/s ²]
Particle diameter	d_p	3×10^{-4}	[m]
Particle terminal velocity	U_t	1.179	[m/s]
Minimum fluidization velocity	U_{mf}	0.0265	[m/s]
Superficial velocity	U_0	0.2	[m/s]
Ratio U_0/U_{mf}	U_0/U_{mf}	7.54	[-]
Number of particles case 1	N_p	1024	[-]
Number of particles cases 2A, 2B	N_p	2304	[-]
Normal restitution coefficient	e_n	0.97	[-]
Tangential restitution coefficient	e_t	0.39	[-]
Coulomb's friction coefficient	μ_c	0.4	[-]
Domain size case 1	$L_x \times L_y \times L_z$	$8d_p \times 8d_p \times 64d_p$	[m ³]
Domain size cases 2A, 2B	$L_x \times L_y \times L_z$	$12d_p \times 12d_p \times 64d_p$	[m ³]
Resolution	$N_d = \frac{d_p}{h}$	16	[-]
Time step	Δt	1×10^{-6}	[s]
Density ratio	ρ_r	1000	[-]
Particle Reynolds number	Re_p	3	[-]
Froude number	Fr	13.6	[-]
Stokes number	St_k	166.7	[-]

Table 4.10: Resolved simulations of gas-solid fluidized beds: physical and numerical parameters.

These observations indicate that, although the two systems of particles are equivalent in an average sense, the dimension of the computational domain in the transverse directions has a dramatic effect on the dynamics of the bed. As noted in [35], the size of the domain, in particular in the transverse dimensions, forces the development of specific heterogeneous structures. There exists a minimum domain size above which the flow dynamics is no longer significantly modified if the dimensions are further increased. Clearly, this minimum domain size will depend on the flow regime. Compared to the liquid-solid fluidized beds that we discussed earlier, gas-solid fluidized beds with high density ratios have little damping effects on the emergence of instabilities and their resolved simulation thus requires large transverse dimensions. It is likely that using $L_x = L_y = 12d_p$ in case 2A is not yet sufficient for the problem considered here, but further increasing the transverse dimension of the domain would have been computationally prohibitive. Figure 4.35 shows the dynamics of the bed with solid walls. Note that, on those frames, particles are colored by their vertical velocity component (vs. the norm in Figures 4.34 and 4.35). A recirculation phenomenon is clearly identified,

with particles moving downwards along the wall at the front of the picture. To get more insight about the influence of the side walls on the global hydrodynamic behavior of the bed, we compare in Figure 4.36 the trajectories of four randomly chosen particles in cases 2A and 2B. The recirculation loop in the case with solid walls is evidenced in Figure 4.36d. It can also be observed that the presence of the walls reduces the altitude reached by the particles, i.e. the height of the bed. In the transverse direction, we also notice that particles display more long-range motion than in the bi-periodic case, which is also a consequence of the recirculation zone.

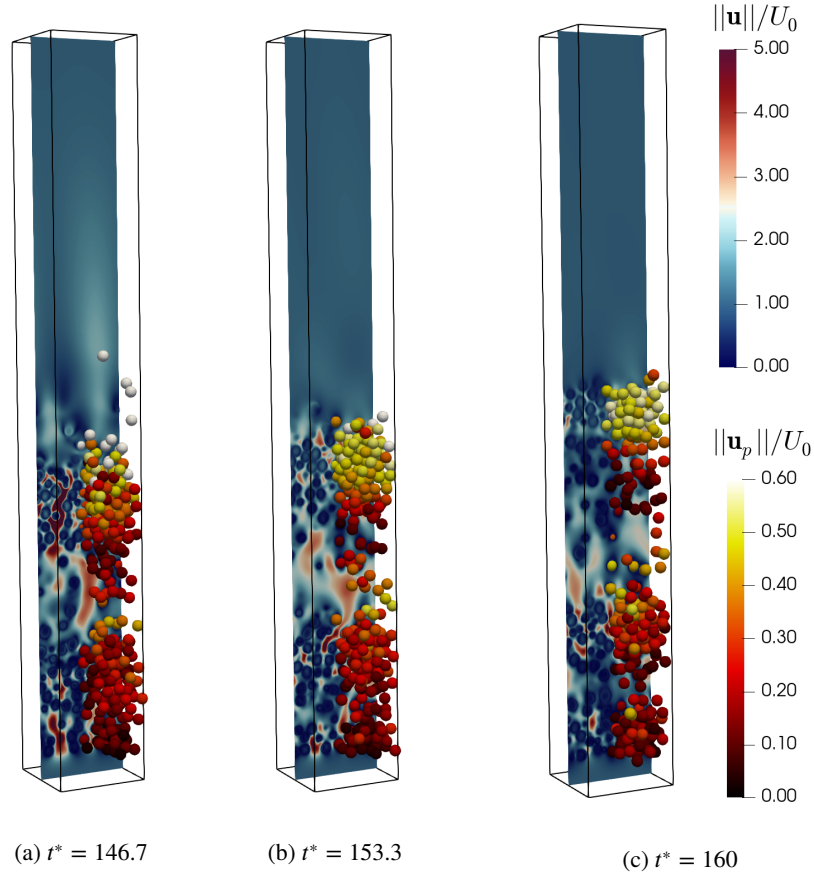


Figure 4.33: Flow dynamics in a bi-periodic gas-solid fluidized bed at $(\text{Re}_p, \rho_r, \text{Fr}) = (3, 1000, 13.6)$ with $N_p = 1024$ particles (case 1), at three successive times.

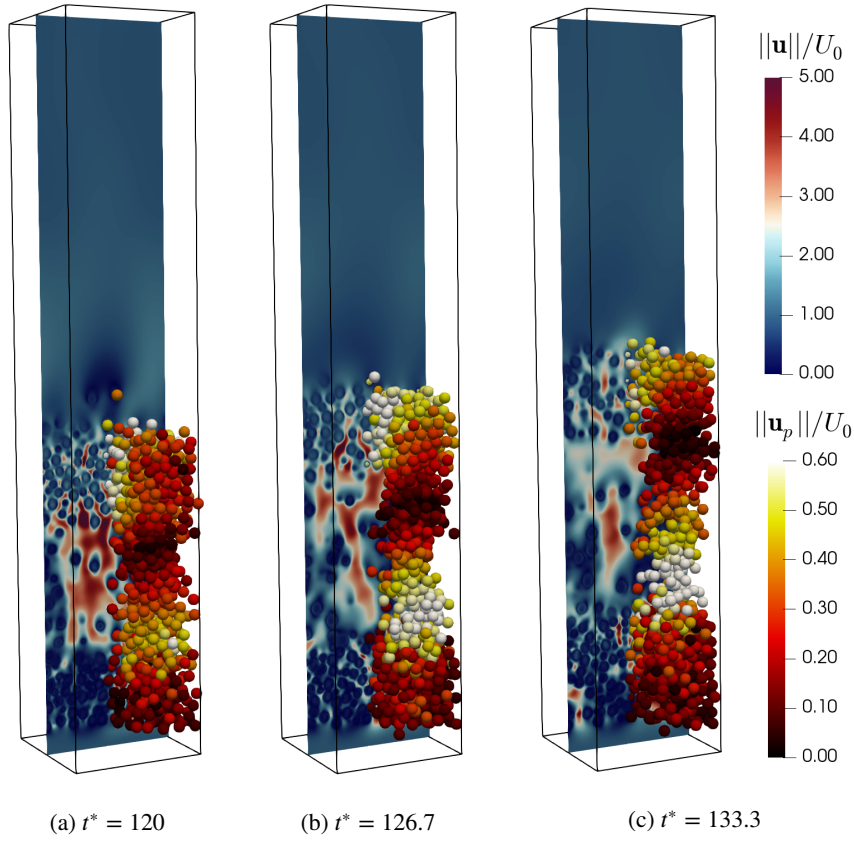


Figure 4.34: Flow dynamics in a bi-periodic gas-solid fluidized bed at $(\text{Re}_p, \rho_r, \text{Fr}) = (3, 1000, 13.6)$ with $N_p = 2304$ particles (case 2A), at three successive times.

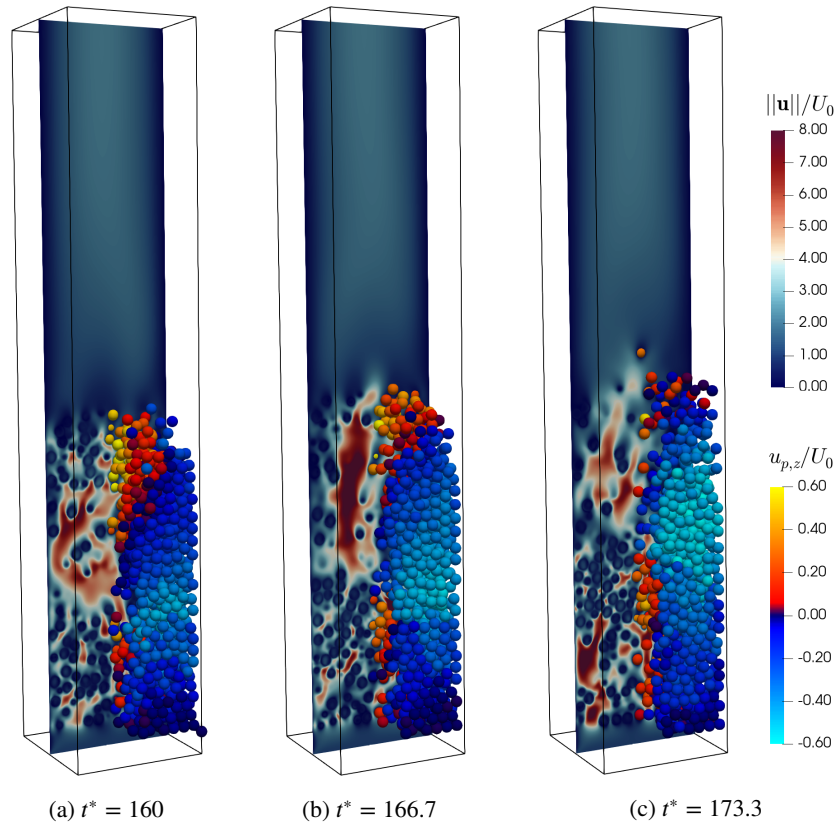


Figure 4.35: Flow dynamics in a gas-solid fluidized bed at $(\text{Re}_p, \rho_r, \text{Fr}) = (3, 1000, 13.6)$ with $N_p = 2304$ particles and solid walls (case 2B), at three successive times.

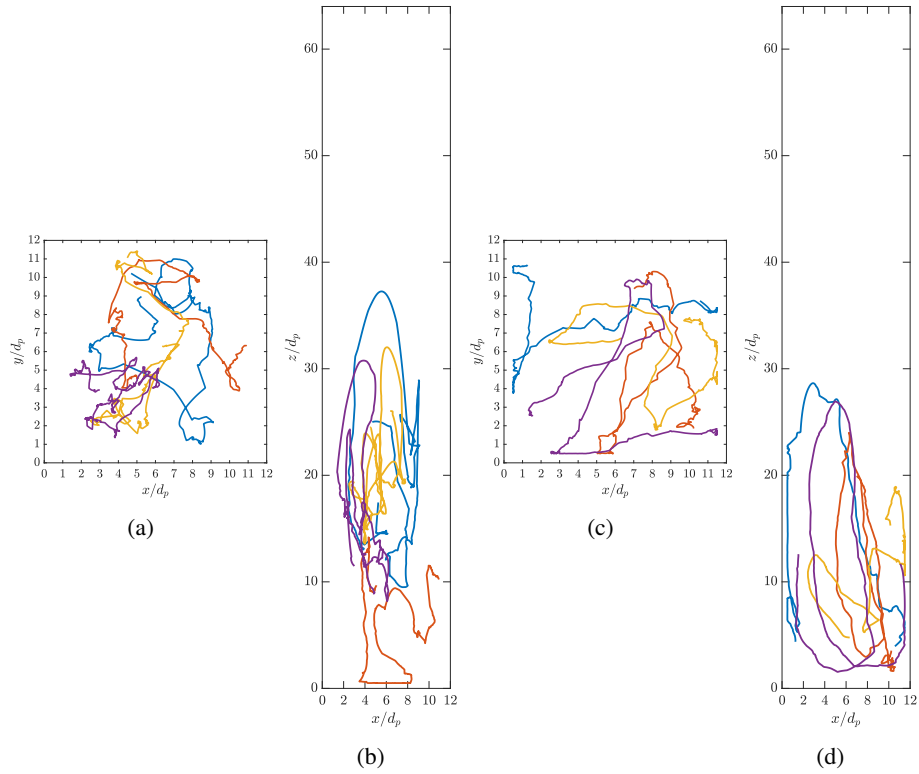


Figure 4.36: Projection of the trajectories of four particles in the transverse plane $z = L_z/2$ and the vertical plane $x = L_x/2$ in case 2A ((a) and (b)) and case 2B ((c) and (d)).

We show in Figure 4.37 the evolution of the bed height for the three cases investigated, using the 99% definition that we introduced earlier. As inferred from Figure 4.33, the case 1 with $N_p = 1024$ particles show strong oscillations around the mean bed height, with peak-to-peak distance exceeding ten diameters. The case 2A ($N_p = 2340$, bi-periodic) also presents an episodic motion but at significantly lower amplitude and slightly higher frequency. Still, these oscillations are much larger than in liquid-solid fluidized beds where bed height fluctuations did not exceed one particle diameter. Finally, the addition of solid walls appears to dampen slightly the oscillations. In the following, time averages will be computed in the interval $t^* \in [70, 310]$ in order to remove the influence of the start-up in the reported statistics. The time averages of the bed height are reported in Table 4.11 for the three cases considered. As expected, case 1 shows excessive expansion. More interestingly, the mean bed height is slightly reduced from case 2A to case 2B, despite the fact that the solid walls limit the size available for the particles in the transverse dimension (particles are no longer free to cross the boundaries). In what follows, we compare cases 2A and 2B in more detail since it appears that case 1 is too constrained to provide relevant results.

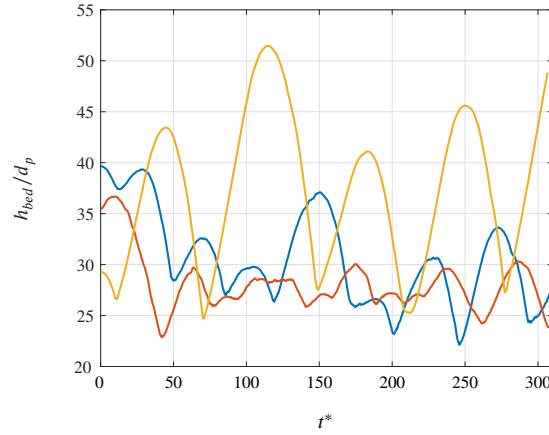


Figure 4.37: Time evolution of the bed height (99% definition) in case 1 (—), case 2A (—) and case 2B (—).

Figure 4.38a compares the time-averaged solid fraction profiles between cases 2A and 2B. First, it can be noted that $\bar{\phi}_s$ is not constant but rather slightly decreases along the bed. This shows that solid particles are slightly more concentrated at the bottom of the bed and that the bubbling phenomenon extends the bed vertically, resulting in

	Case 1	Case 2A	Case 2B
$\bar{h}_{bed}/d_p$	37.8	29.2	27.4

Table 4.11: Mean height of the gas-solid fluidized bed estimated from the 99% definition for the three cases investigated.

a slight negative gradient in the streamwise profile of the time-averaged solid volume fraction. The decrease of the solid volume fraction in the freeboard region is also sharper in the case 2B, which further confirms the damping of the bubbling phenomenon in the presence of solid walls. In Figure 4.38b, the comparison of the time-averaged pressure profile obtained from our simulations with the head losses predicted by Eq. (4.42) shows a good agreement. It can be noted that the total pressure drop is slightly higher in the case 2B due to the resistance of the walls.

4.6.3 Particle velocity statistics

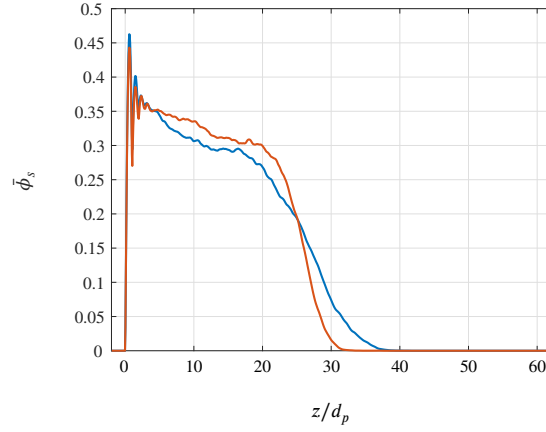
To highlight a little more the recirculation loop phenomenon in the case with solid walls, we compute the average of the vertical velocity component of the particles contained in a vertical slice bounded by the transverse positions $x - \frac{\Delta x}{2}$ and $x + \frac{\Delta x}{2}$, which reads

$$\langle u_{p,z} \rangle_{slice_{\Delta x}}(x, t) = \frac{\sum_{k=1}^{N_p} H(x_p^{(k)}(t), x, \Delta x) u_{p,z}^{(k)}(t)}{\sum_{k=1}^{N_p} H(x_p^{(k)}(t), x, \Delta x)}, \quad (4.69)$$

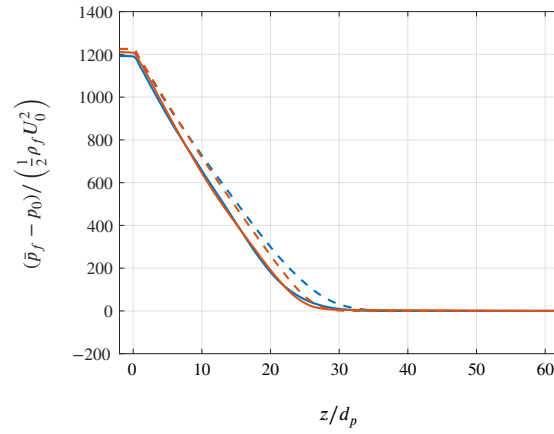
where

$$H(x_p(t), x, \Delta x) = \begin{cases} 1, & x_p \in [x - \frac{\Delta x}{2}, x + \frac{\Delta x}{2}], \\ 0, & \text{otherwise.} \end{cases} \quad (4.70)$$

Then, we further average this quantity in time to get the time-averaged profile $\langle u_{p,z} \rangle_{slice_{\Delta x}, t}$ shown in Figure 4.39a. The same procedure is repeated in the y direction in Figure 4.39b. It can be observed that in the case 2B, particles take negative velocities close to the left wall in the x direction ($x = 0$) and positive values close to the right wall ($x = L_x$). This shows that the recirculation loop has its "angular velocity vector" oriented in the y direction, although nothing would have prevented the recirculation loop to establish in the other transverse direction, given the symmetry of the problem. In the bi-periodic case, particles appear to exhibit positive vertical velocities in the middle of the domain in the x direction, with the time averaging done here from $t^* > 70$, and negative values close to the periodic boundaries, while the vertical velocity profile in the y direction (Figure 4.39b) is fairly flat. This tends to show that the bubbling phenomenon in the case 2A induces some transverse anisotropy, at least



(a)



(b)

Figure 4.38: (a) Time-averaged solid volume fraction profile and (b) time-averaged pressure profile (bottom) in case 2A (—) and case 2B (—). The pressure profiles are compared to the theoretical head losses given by Eq. (4.42) (--- and ---, respectively).

when averaged over the time of the simulation and when constrained by the present bi-periodic domain. It remains to be seen if that would still be the case if the domain was larger. Yet, it must be noted that the values in Figure 4.39 are about two orders

of magnitude smaller than the mean level of particle velocity fluctuations presented in the next section. Ozel et al. [95] also identified a recirculation loop in their resolved simulation of a liquid-solid fluidized bed with solid walls, but the geometry of the vessel was cylindrical so that these authors observed an axisymmetric recirculation loop with particles rising at the center of the domain and moving downward along the side walls.

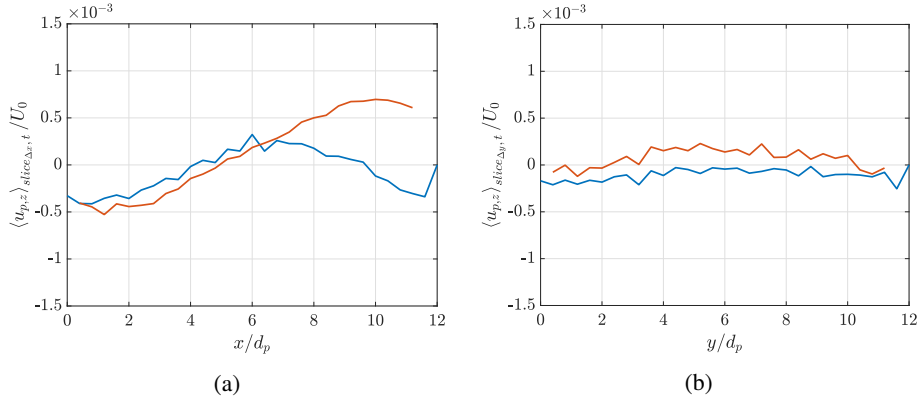


Figure 4.39: Time average of the mean vertical velocity component computed in vertical slices along the (a) x and (b) y directions in case 2A (—) and case 2B (—).

The instantaneous mean of the vertical component of particle velocity shown in Figure 4.40a highlights the strong oscillatory motion of the fluidized bed in the vertical direction, and the impact of the side walls on its mitigation (case 2B). In the transverse direction (Figure 4.40b), the mean value is virtually zero for all times in case 2A, while it shows some oscillations in case 2B. Figures 4.40c and 4.40d show the time evolution of the standard deviation of particle velocity in the vertical and transverse directions, respectively. The mean level of velocity fluctuations is significantly lower than in the case of liquid-solid fluidized beds (see Figure 4.16c and 4.16d). The same finding was reported by Esteghamatian et al. [36], despite the fact that, in their study, the liquid-solid fluidized bed was characterized by a smaller Reynolds number than the gas-solid fluidized bed, contrary to our work. This tends to demonstrate that the agitation is not primarily driven by the Reynolds number but rather by the inertia of the solid particles, i.e. the Stokes number. Highly inertial particles take time to modify their motion and adapt to fluctuations in the flow field, which explains the smaller level of fluctuations in particle velocity. Similar conclusions were drawn by Tenneti et al. [131] and Tang et al. [123]. However, the anisotropy coefficient defined by Eq. (4.37)

increases to $K_U = 2.67$ for the case 2A and $K_U = 2.37$ for the case 2B, showing the larger influence of the mean flow on the motion of the solid particles in a gas-solid fluidized bed with respect to the liquid-solid case.

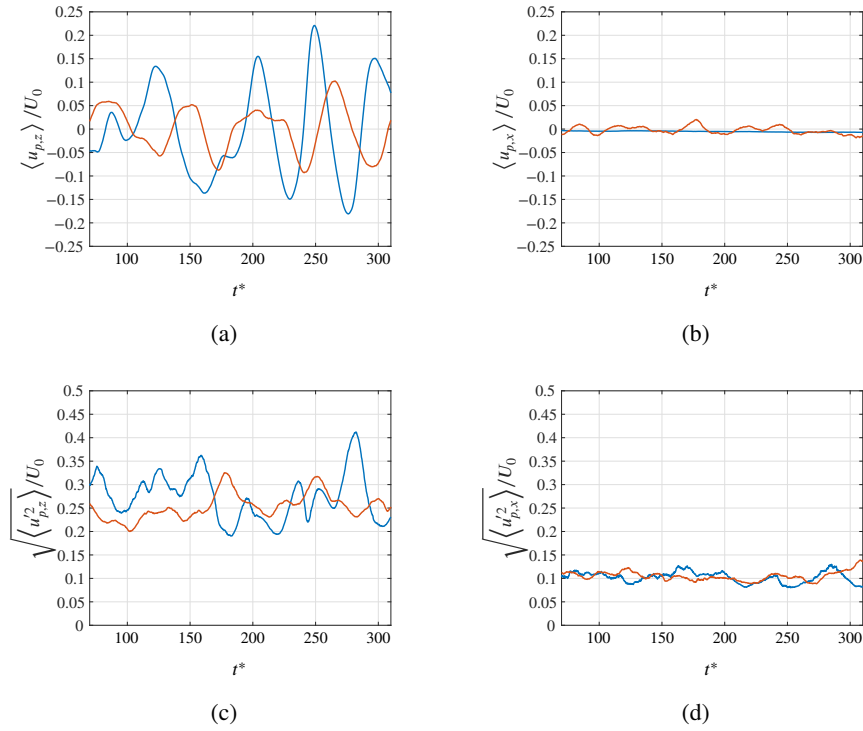


Figure 4.40: Time evolution of (a) the mean vertical component, (b) the mean transverse component, (c) the standard deviation of the vertical component and (d) the standard deviation of the transverse component of particle velocity in case 2A (—) and case 2B (—).

We examine again the behavior of the particle velocity auto-correlation function, $R_{U_i U_i}$, shown in Figure 4.41. In case 2A, the auto-correlation function in the vertical direction shows a negative minimum and then oscillates before converging to zero for large time lags, which confirms the superposition of an oscillatory motion induced by the mean flow and an intrinsic diffusive motion. In the transverse direction, the auto-correlation function first decays very fast, and then decreases slowly towards zero in an exponential fashion. For the case 2A, the correlation time and length scales in the transverse and vertical directions are given in Table 4.12. Correlation time scales

take significantly larger values than in liquid-solid fluidized beds, showing the larger influence of the vertical advective motions in gas-solid fluidized beds. It can be observed in Figure 4.41 that the presence of solid walls drastically modifies the shape of the auto-correlation functions. In case 2B, both $R_{U_x U_x}$ and $R_{U_z U_z}$ display a low-frequency oscillatory motion which appears as a clear signature of the recirculation phenomenon. In fact, the definition of the Lagrangian fluctuation that we introduced in Eq. (4.30) does not allow us to extract the part of the velocity that is independent of the large-scale collective motion induced by the recirculation loop. In other words, the recirculation motion is visible in the particle velocity fluctuations while it does not reflect the actual agitation level in the bed. If we were trying to get rid of this contribution, we should determine the local time average of the particle velocity at a specific point in space. Hence, we do not provide correlation time and length scales for case 2B.

$\tau_{U_x}^*$	$\tau_{U_z}^*$	$l_{U_x}^*$	$l_{U_z}^*$
9.66	8.13	0.96	2.16

Table 4.12: Particle velocity correlation time and lengths scales in case 2A.

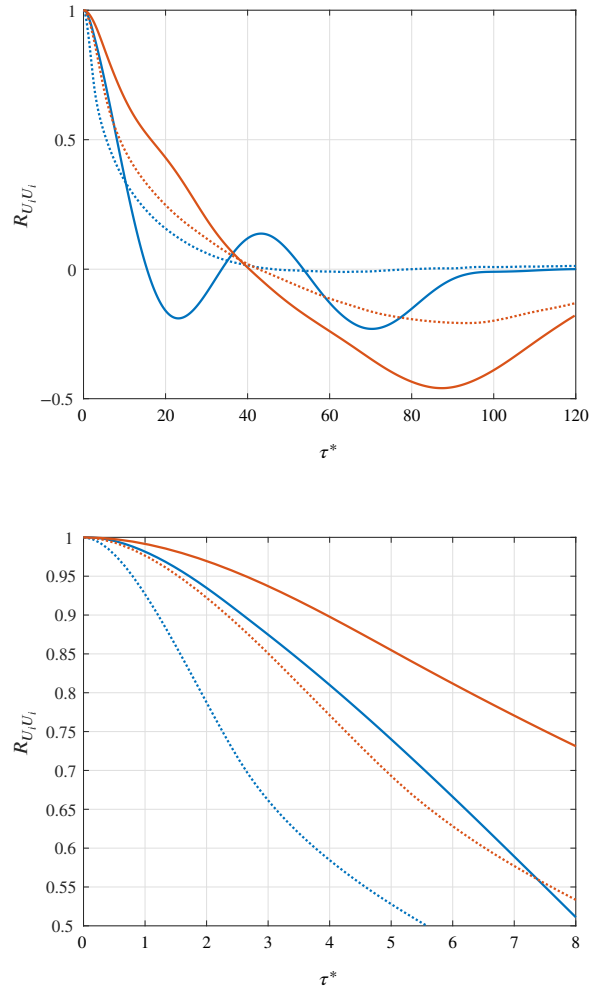


Figure 4.41: Global (top) and close-up view (bottom) of the particle velocity auto-correlation function in the vertical (solid) and transverse (dotted) directions in case 2A (—, ···) and case 2B (—, ···).

4.6.4 Force statistics

Let us now examine the statistics of the fluid-particle force. In Table 4.13, we compare the normalized mean vertical component of the fluid-particle force obtained from our resolved simulations to the values predicted using a few correlations from the literature. To that end, we had to determine the mean porosity of the bed. Since the time-averaged solid volume fraction profiles in Figure 4.38a do not show a clear plateau, the mean solid volume fraction is estimated as $\phi_s = \frac{N_p V_p}{h_{bed} S}$, using the time-averaged bed heights reported in Table 4.11. We also introduced in Table 4.13 the "dynamic" correlation of Tang et al. [123] that was proposed following the observation that the mean drag force measured in moving gas-solid suspensions was significantly larger than the values provided by commonly used drag laws. This dynamic correlation is built from the original drag law proposed by Tang et al. [124] as

$$\bar{F} = \bar{F}_{Tang}(\text{Table 2.1}) + 2.98 \text{Re}_T \frac{\phi_s}{(1 - \phi_s)^3} \quad (4.71)$$

where Re_T is the thermal Reynolds number defined as

$$\text{Re}_T = \frac{\rho_f d_p \sqrt{\Theta}}{\mu} \quad (4.72)$$

and where Θ is the average granular temperature of the system:

$$\Theta = \frac{1}{3} \left(\left\langle u'_{p,x} u'_{p,x} \right\rangle_t + \left\langle u'_{p,y} u'_{p,y} \right\rangle_t + \left\langle u'_{p,z} u'_{p,z} \right\rangle_t \right). \quad (4.73)$$

The thermal Reynolds number happens to be identical in cases 2A and 2B and equal to $\text{Re}_T = 0.53$.

For the case 2A, as reported by several authors [68, 124], we observe in Table 4.13 that the drag laws derived from resolved simulations in static particle arrays underestimate the mean fluid-particle force in the vertical direction. Interestingly, the dynamic correlation of Tang et al. [123] (last column in Table 4.13) significantly improves the prediction. A question that arises is to know why we observe this increase in the drag force in gas-solid suspensions (with respect to the static case) while we did not observe it in liquid-solid suspensions. Tavanashad et al. [125] addressed this question in a recent work [125]. These authors showed that when we move from a homogeneously distributed static array to a free suspension, three different phenomena impact the mean fluid-particle force: the clustering of particles, the mobility, i.e. the possibility for a particle to adapt its motion to the streamlines of the flow, and the level of agitation due to the fluctuations in particle velocities. Tavanashad et al. [125] showed that the

mobility of the particles decreases the mean hydrodynamic force since particles can adapt their motion to reduce the net stresses on their surface. Rubinstein et al. [108] previously drew the same conclusions in Stokes regime. Conversely, particle velocity fluctuations increase the mean fluid-particle force, and this effect increases with the Reynolds number and decreases with the density ratio. The clustering of particles can have different effects depending on whether the clusters have a vertical shape aligned with the flow (decrease of the drag) or a horizontal shape perpendicular to the flow (increase of the drag). In the latter case, particles are usually organized in "rafts" at the top of the rising bubbles. The mobility of the particles and their ability to adapt to the streamlines of the flow is higher as the Stokes number of the suspension decreases. Hence, it appears that in the case of liquid-solid fluidized beds, in the absence of clusters, the impact of the particle velocity fluctuations on the fluid-particle force is somehow counterbalanced by the high mobility of the solid particles in the fluid. In gas-solid fluidized beds, although the level of velocity fluctuations is lower than in the liquid-solid case, the formation of raft clusters above the bubbles and the lower mobility of the particles result in an increase of the fluid-particle force. The relative contribution of each of these effects is, however, hard to establish.

For the case 2B, although the bed is slightly more dense and the Reynolds number is identical, we report a slightly smaller value for $\langle F_{p,z} \rangle$. This finding might be attributed to the collective motion of the particles inside the recirculation loop resulting in a lower resistance to the flow.

	Present	Tenneti [134]	Beetstra [9]	Tang [124]	Tang (dyn.) [123]
Case 2A	11.87	9.79	9.81	10.65	11.95
Case 2B	11.52	11.20	11.20	12.16	13.67

Table 4.13: Normalized mean vertical component of the fluid-particle force $\bar{F} = \langle F_{p,z} \rangle_t / F_{St}$ in gas-solid fluidized beds.

The fluid-particle force auto-correlation function presented in Figure 4.42 shows a similar behavior as the particle velocity auto-correlation function. For the case 2A, the auto-correlation function in the vertical direction shows strong oscillations before converging towards zero while in the transverse direction, $R_{U_x U_x}$ decays rapidly towards zero, yet showing a negative minimum. The correlation time and length scales of the fluid-particle force are given for the case 2A in Table 4.14.

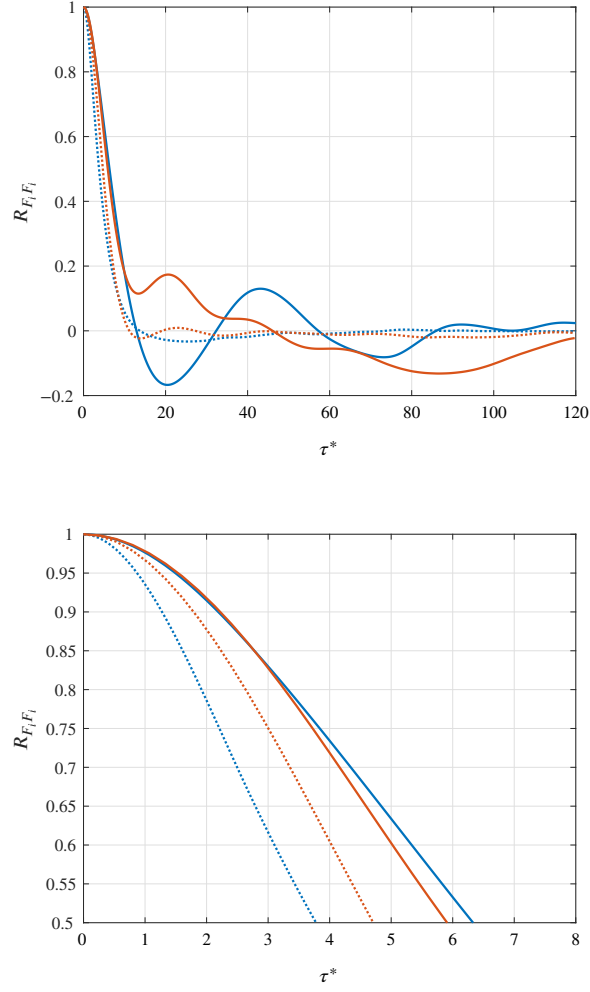


Figure 4.42: Global (top) and close-up view (bottom) of the fluid-particle force auto-correlation function in the vertical (solid) and transverse (dotted) directions in case 2A (—, ···) and case 2B (—, ···).

$\tau_{F_x}^*$	$\tau_{F_z}^*$
4.44	6.49

Table 4.14: Fluid-particle force correlation time scales in case 2A.

4.7 Conclusions

This study investigated the dynamics of fluidized beds in different regimes using particle-resolved simulations. We first examined the settling of a homogeneous suspension in a 3-D periodic box in presence of an adverse pressure gradient to cancel the net fluid flow rate. This first problem showed the capability of our method to handle flows with moving particles and yield faithful results. By changing the number of solid particles in the box, we were able to characterize the influence of the solid volume fraction on the mean settling velocity and on the level of fluctuations.

Then, we performed resolved simulations of liquid-solid fluidized beds at three different superficial velocities. We first investigated the global hydrodynamics of the bed. In those regimes, a smooth and homogeneous fluidization is observed, without the emergence of bubbles or clusters. However, a significant anisotropy is identified between the vertical and the transverse directions, owing to the influence of the mean flow. We also studied the influence of the fluidization velocity on the mean bed porosity and our results were compared to the well-known Richardson-Zaki's law. In a log-log diagram, we recover the linear relation between the fluidization velocity and the void fraction, but, as observed in previous studies, the extrapolation of the fluidization velocity at infinite dilution is significantly lower than the terminal velocity U_t . Then, Lagrangian statistics were analyzed in details. In particular, auto-correlation functions were computed for the particle velocity and the fluid-particle force, showing the superposition of a diffusive motion related to the agitation of the bed and an oscillatory motion induced by the large-scale structures. It was also demonstrated that the mean square displacement and the Lagrangian correlation time scale evaluated from the particle velocity auto-correlation functions produce fairly similar results for the self-diffusion coefficient. Next, we examined the distribution of the fluid-particle force. It was shown that the mean vertical component of the fluid-particle force compensates correctly the buoyancy force, by definition of the fluidized state, and is fairly well predicted by correlations derived from PR-DNS on static particle arrays. We also demonstrated that the shape of the pdf of the force in homogeneous fluidized beds is similar to the fixed bed case, except for values far from the average. In those regions, it was shown that the pdf of the force has a "heavy tailed" behavior and follows a power law. Finally, the thermal problem was addressed. The mean Nusselt number extracted from a control volume in the homogeneous region of the bed appears to be slightly larger than the values predicted by the correlations derived from the flow past non-isothermal fixed particle arrays. As observed in Chapter 3, thermal saturation occurs

faster as the bed is dense and the particle Reynolds number is low, giving a skewed shape to the heat flux distributions.

In a last section, we studied the dynamics of gas-solid fluidized beds. The much greater inertia of the solid particles in these systems leads to the emergence of an intense bubbling phenomenon and to an episodic motion of the bed. We showed that the transverse dimension of the domain is an important factor as it determines the size of the heterogeneous structures that emerge in the bed and, consequently, the intensity of the oscillatory motion. Then, we investigated the impact of using solid walls in the transverse directions. The dynamics of the bed appears to be drastically modified, with the emergence of a recirculation loop. Furthermore, the oscillatory motion of the bed appears to be significantly attenuated. The auto-correlation functions show that, in the bi-periodic case, we recover the superposition of a decaying pseudo-random motion and an oscillatory motion in the vertical direction, the latter being much more intense than in liquid-solid fluidized beds. In the transverse direction, however, the particle velocity auto-correlation function decays smoothly towards zero. In addition, the particle velocity anisotropy coefficient appears to be significantly larger in gas-solid than in liquid-solid fluidized beds. In the case with solid walls, particle velocities stay correlated for very long times, owing to the spatial correlation introduced by the recirculation loop that is not accounted for in the definition of the fluctuations. Finally, we confirmed previous observations from the literature claiming that the mean vertical fluid-particle force in gas-solid suspensions is underestimated by drag laws derived from resolved simulations in fixed particle arrays.

In the future, we should perform resolved simulations of liquid-solid and gas-solid fluidized beds in a larger range of superficial velocities. Doing so, we would be able to better identify the relative influence of the Reynolds and Stokes numbers on the dynamics of the fluidized beds. This would also allow us to study in more details the influence of the bed agitation on the mean drag force experienced by the particles and on the mean fluid-particle heat flux. Next, we could apply the microstructure-based methodology developed in Chapter 2 to the case of moving particles in fluidized beds. Since fixed arrays of particles correspond to systems with an infinite Stokes number, it is expected that the model developed in Chapter 2 will show better performance in gas-solid fluidized beds than in liquid-solid fluidized beds. Nevertheless, we should repeat the search for existing correlations between the fluid-particle force and microstructure-based tensor quantities, even those that have been excluded from the original model. Also, the correlation time scales computed from the fluid-particle force auto-correlation functions could be used to estimate the time scale to give to the isotropic Gaussian noise in the stochastic version of our microstructure-based model

for a future use in a CFD-DEM framework. Finally, we should study the behavior of the auto-correlation function calculated from the decorrelated particle velocities. Doing so, we would be able to separate the diffusive motion of the particles from the collective motions that appear in the bed (e.g. oscillatory motions, recirculation zones,...).

Conclusions

This thesis was dedicated to the direct numerical simulation of fluid-particle flows. Particle-laden flows offer a rich variety of flow regimes that can be considered to be controlled by three main factors: the dilution of the dispersed phase, the momentum transfer driving force (i.e. the slip velocity between the two phases) and the inertia of the solid particles in the carrier fluid (i.e. their ability to adapt their motion to changes in the flow field). Although still limited to small-scale systems because of the large computational resources it requires, PR-DNS offers the most refined level of flow details. In the past decades, it has emerged as the tool of choice to quantify unclosed terms in larger-scale approaches, namely the unresolved Euler-Lagrange and the Euler-Euler methods.

Our work was two-fold. A first part of this work was dedicated to the development and validation of a numerical method to be able to perform accurate and reliable particle resolved simulations in three dimensions. In a second part, the methodology was applied to the study of the flow past static arrays of particles and to freely evolving suspensions, namely liquid-solid and gas-solid fluidized beds. In what follows, we first highlight the main results obtained in the different chapters of this thesis. Finally, we discuss the potential improvements and research areas for future investigations.

Achievements

In Chapter 1, we developed a direct-forcing immersed boundary method based on the formulation proposed by Breugem [15]. The methodology was first developed in a 2-D and then in a 3-D framework. The enforcement of Dirichlet boundary conditions is ensured by the addition of a forcing term in the governing equations of the fluid. This

forcing term is first evaluated on a collection of Lagrangian points distributed on the surface of the particles before being interpolated on the Cartesian grid. The retraction of the Lagrangian points from the physical surface is needed to avoid an overestimation of the hydrodynamic radius and the retraction distance appears to be a determining factor in the accuracy of the results produced by the method. The spatial accuracy of the method was proved to be between first and second order. The methodology was also extended to handle heat and mass transfer phenomena and to couple the motion of the particles with natural convection effects. Finally, the master-slave parallelization strategy of our combined immersed boundary/discrete element method was detailed and dedicated studies showed the good scaling performance of the complete 3-D solver.

In Chapter 2, we investigated the distribution of the fluid-particle force in the flow past statistically homogeneous random arrays of particles, highlighting the significant dispersion of the force around its mean value. To predict part of the variability of the force in the particle array, we characterized the microstructure formed by a reference particle and its near neighbors using tensor quantities inspired from the so-called fabric tensor used in granular media. Significant correlations were identified between some microstructure characteristic quantities and the components of the fluid-particle force. A deterministic microstructure-based multi-linear model was then proposed. It was shown to perform better in predicting the streamwise component of the force in the dense and viscous regimes. This deterministic model was found to underestimate the level of fluctuations of the force. Therefore, a stochastic contribution was added to the initial deterministic model. We showed that the correct level of fluctuations can be recovered by this stochastic model at the cost of a lower correlation between the model and the data.

Chapter 3 was dedicated to the study of the heat transfer in the flow past fixed particle arrays. We first discussed the analogy with the heat transfer in a pipe flow and the thermal saturation problem. Then, we showed how our PR-DNS data could be used to estimate the unclosed mean interfacial heat flux and pseudo-turbulent heat flux terms in the Euler-Euler energy equation. Next, we examined the distribution of the fluid-particle heat flux among the particles and we highlighted its skewness in regimes where thermal saturation occurs fast, i.e. dense and viscous regimes. It was then shown that the particle Nusselt number presents a more symmetric distribution and that it is statistically homogeneous in the streamwise direction. Finally, a preliminary study showed that the correlation between the particle Nusselt number and the microstructure characteristic quantities retained in the model of the streamwise fluid-particle force was non-zero, but much weaker, hence requiring further investigation.

Finally, Chapter 4 was dedicated to the study of freely evolving suspensions. We first examined the settling of homogeneous suspensions in presence of an adverse pressure gradient. This first problem confirmed the capacity of our method to handle particle flows in dense and dilute regimes, and to yield faithful results. We then focused on small-scale fluidized beds. We first performed resolved simulations of bi-periodic liquid-solid fluidized beds at different superficial velocities and we investigated in details the hydrodynamics of the bed. As the superficial velocity increases, the bed expands homogeneously and a fluidization law in line with Richardson-Zaki's original relation is obtained. The Lagrangian statistics of the particles were also examined. The diffusive motion of the particles was characterized from their mean square displacement and using the particle velocity auto-correlation function. Then, the distribution of the fluid-particle force was analyzed in details. The mean value of the force was found to correctly counterbalance the buoyancy force and to be fairly well predicted by correlations used for fixed particle arrays. It was also shown that the shape of the force distribution in its main part is similar in the cases of fixed and fluidized beds. For large values of the force, the pdf in the fluidized bed case decreases much more slowly than in the fixed bed case and follows a power law distribution. The thermal problem was also addressed. The mean Nusselt number extracted from a control volume in the core of the bed showed a fairly good agreement with the correlations derived from static particle arrays. We observed a slight enhancement of the heat transfer as the superficial velocity increases although the reason behind this finding is not clear. We also demonstrated that the distributions of the fluid-particle heat flux and particle Nusselt number exhibit a significant skewness in the three regimes investigated. Finally we studied gas-solid fluidized beds characterized by a much larger solid-fluid density ratio (and therefore a larger Stokes number). The strong inertia of the solid particles in such systems leads to the emergence of heterogeneous structures, namely gas bubbles and clusters of particles. We highlighted the stronger anisotropy of the particle motion in gas-solid fluidized beds and the larger influence of the mean flow and advective motions with respect to the liquid-solid case. It was also shown that the dimensions and the type of boundary conditions in the transverse directions can have dramatic effects on the dynamics of the bed. In particular, the presence of solid walls induces the establishment of a recirculation loop in one of the transverse directions which is found to dampen the oscillatory motion of the bed. Contrary to liquid-solid fluidized beds, we report larger values for the mean fluid-particle force than those obtained from usual drag laws. The relative contributions to this increase (mobility, agitation and clustering) are difficult to establish, though.

Perspectives

Several improvements and further investigations are being considered, both regarding the numerical method developed in this work and the exploitation of the results.

On the numerical method

The direct-forcing immersed boundary method developed in this work has been efficiently used to perform resolved simulations of fairly large systems (from a DNS perspective). Yet, as previously mentioned, the need to retract the Lagrangian points from the surface appears as a weakness of the method. A possible cure to get rid of this arbitrary parameter would be to replace the symmetric Roma's interpolation kernel [106] currently used in our simulations by an asymmetric quadratic interpolation operator such as proposed by Wachs et al. [148] in their DLM/FD method. Another formulation that we could consider and that prevents the overestimation of the hydrodynamic radius is the PReIBM method of Subramaniam and co-workers [132, 134, 133, 120, 121]. In both cases, the knowledge of the local outwards normal vector at the particle boundary is required to construct the interpolation operator and evaluate the forcing term. Another issue is the weak coupling between the solid and the fluid phases due to the staggered advancement of the fluid and solid phase motions. While we showed that the present method is stable down to a solid-fluid density ratio $\rho_r \geq 1$, the current formulation could lead to instabilities if we were targeting particles lighter than the carrier fluid or bubbles in a liquid. The fully implicit (i.e. strong) coupling of the two phases would require an iterative procedure to simultaneously update the new position of the interface, its velocity, and the velocity of the fluid. Recently, Tschisgale et al. [137] developed a semi-implicit IBM that avoids to iterate on the complete solver, which appears as a interesting compromise that we could examine.

Our method is currently limited to monodisperse spherical particles. The inclusion of polydispersity (i.e. particles of different sizes) in our solver should be a fairly easy task in the near future. The handling of non-spherical particles in the current framework will require some more work for at least two reasons : (i) the non-obvious retraction of the Lagrangian points from the surface of non-spherical objects, especially angular solids (e.g. cubes) (ii) the more complex search for collisions in three dimensions. In any case, polydispersity appears to be the most interesting and pressing issue as it has been shown to have a significant impact on the average fluid-particle force [156, 115] and therefore on the dynamics of the bed.

In the future, we would like to perform 3-D resolved simulations of reacting gas-solid flows with coupled heat and mass transfer between the solid and the fluid phases

by solving the intra-particle temperature and species mass fraction gradients. Actually, this work has already been initiated in 2-D by coupling our IBM with a sharp interface method for the scalar fields (see Appendix E) and we aim to extend this approach to our 3-D solver. Still with the idea of studying reacting gas-solid flows, we would like to extend the current methodology to a weakly compressible (i.e. variable density) framework. We started to address this issue in a Brinkman penalization framework (see Appendix F), although some fundamental questions are still open regarding the validity to consider a fluid with variable density inside the solid particles.

On the modeling and the physics of fluid-particle flows

From a modeling perspective, a first challenge will be to improve our microstructure-based model developed in Chapter 2 in static particle arrays. We showed that the performance of the model deteriorates as we move towards more inertial and dilute regimes. The current model relies on a few parameters (width of the Gaussian filter, cutoff distance) that are currently not dependent on the flow regime. A fine tuning of those parameters in order to optimize its performance would be of great interest for a future deployment into a CFD-DEM framework.

We should also further investigate how the distribution of the fluid-particle force evolves in freely evolving suspensions, for a wide range of flow parameters and in different regimes. In the case of gas-solid fluidized beds, we should deepen our analysis since the results we presented were probably conditioned by the transverse dimensions of the domain in the bi-periodic case and we only examined one fluidization regime. Next, we could repeat the approach of Chapter 2 and examine how the fluid-particle force correlates with microstructure characteristic quantities when particles are free to move. As mentioned earlier, it is expected that the conclusions drawn from our study on static configurations (i.e. at infinite Stokes number) will better match the behavior of gas-solid suspensions with a high Stokes number than liquid-solid suspensions in which the response time of the particles is much shorter. However, the emergence of heterogeneous structures in gas-solid fluidized beds might complicate the analysis.

Regarding the stochastic version of our model, the fluid-particle force correlation time scale extracted from our resolved simulations could be used to estimate the appropriate time scale to provide to the Gaussian noise term, e.g. if we were to model the fluctuating part of the drag as an Auto-Regressive (AR-1) signal such as proposed in [35]. However, a limited number of flow regimes have been investigated. Hence, we should build a larger database of freely moving suspensions for a wide range of parameters (solid fraction, particle Reynolds number, Stokes number). To that end, we might

consider studying suspensions in smaller tri-periodic boxes instead of actual fluidized beds. Those smaller scale systems would allow us to evaluate more systematically the influence of the different flow parameters on the distribution of the fluid-particle force and on its relation to the local microstructure. The final goal will be to actually implement our microstructure-based model in a CFD-DEM framework and to evaluate its performance.

About heat transfer, we would first like to unveil the reasons of some of the discrepancies identified in Chapter 3 regarding the evaluation of the mean interfacial heat flux and the pseudo-turbulent heat flux in some regimes. While our results for the fluid-particle force are in very good agreement with previous studies, a larger variability is observed on our results for the thermal problem. To remove the influence of the thermal entrance in our analyses, we could consider the self-similarity method developed by Tenneti et al. [134] and therefore perform resolved simulations of fluid-particle flows with heat transfer in tri-periodic domains.

Then, we should further investigate the relation between the fluid-particle heat flux and the organization of the microstructure. A preliminary study showed the rather limited correlation between the (statistically homogeneous) particle Nusselt number and the quantities retained for the modeling of the streamwise component of the fluid-particle force, showing the limits of the analogy between momentum and heat transfer. Clearly, a more in-depth analysis is required, including the search for correlations with microstructure quantities that were not retained in the original model and possibly a new calibration of the model parameters tailored to the thermal problem. Another alternative would be to define a Nusselt number based on the locally averaged fluid-phase temperature around each particle and to seek for existing correlations with microstructure characteristic quantities.

This thesis only offered a small glimpse of the rich variety of phenomena produced by particle-laden flows, and their complexity is still far from being fully captured by the human knowledge. With the help of growing computing power, particle resolved simulation should still play a key role in the future towards a more comprehensive understanding of these flows.

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Collision modeling

A.1 Hard-sphere model

The hard-sphere model is an "event-driven" model, in the sense that collisions are treated as discrete events where pre- and post-collision quantities are well defined. On the contrary, the soft-sphere model presented later (and used in our immersed boundary method) is a "time-driven" model where collisions are treated as continuous events and have a finite duration.

Let us consider two colliding particles 1 and 2 as illustrated in Figure A.1. The conservation of linear and angular momentum before and after the contact reads

$$m_1(\mathbf{u}'_1 - \mathbf{u}_1) = \mathbf{J} \quad (\text{A.1})$$

$$m_2(\mathbf{u}'_2 - \mathbf{u}_2) = -\mathbf{J} \quad (\text{A.2})$$

$$I_1(\boldsymbol{\Omega}'_1 - \boldsymbol{\Omega}_1) = R_1 \mathbf{n}_{12} \wedge \mathbf{J} \quad (\text{A.3})$$

$$I_2(\boldsymbol{\Omega}'_2 - \boldsymbol{\Omega}_2) = R_2 \mathbf{n}_{12} \wedge \mathbf{J}, \quad (\text{A.4})$$

where $\mathbf{n}_{12}$ is the unit normal vector pointing from particle 1 to particle 2,

$$\mathbf{n}_{12} = -\frac{\mathbf{x}_1 - \mathbf{x}_2}{\|\mathbf{x}_1 - \mathbf{x}_2\|}, \quad (\text{A.5})$$

$\mathbf{J}$ is the impulse transferred from particle 2 to particle 1 during the collision process and $I = \frac{2}{5}mR^2$ is the moment of inertia of a sphere. The " ' " symbol indicates the post-collision quantities. The five vector unknowns of the problem are the linear and angular velocities of the two particles after the collision and the associated impulse vector. The contact point relative velocity just before the collision is given by

$$\mathbf{u}_{12} = \mathbf{u}_1 - \mathbf{u}_2 + R_1(\boldsymbol{\Omega}_1 \wedge \mathbf{n}_{12}) + R_2(\boldsymbol{\Omega}_2 \wedge \mathbf{n}_{12}). \quad (\text{A.6})$$

The normal and tangential components of the contact point velocity are defined as

$$\mathbf{u}_{12,n} = (\mathbf{u}_{12} \cdot \mathbf{n}_{12})\mathbf{n}_{12}, \quad (\text{A.7})$$

$$\mathbf{u}_{12,t} = \mathbf{u}_{12} - (\mathbf{u}_{12} \cdot \mathbf{n}_{12})\mathbf{n}_{12}. \quad (\text{A.8})$$

The impulse vector is also decomposed into normal and tangential components,

$$\mathbf{J} = J_n \mathbf{n}_{12} + J_t \mathbf{t}_{12}, \quad (\text{A.9})$$

with the unit tangential vector defined as

$$\mathbf{t}_{12} = \frac{\mathbf{u}_{12,t}}{\|\mathbf{u}_{12,t}\|}. \quad (\text{A.10})$$

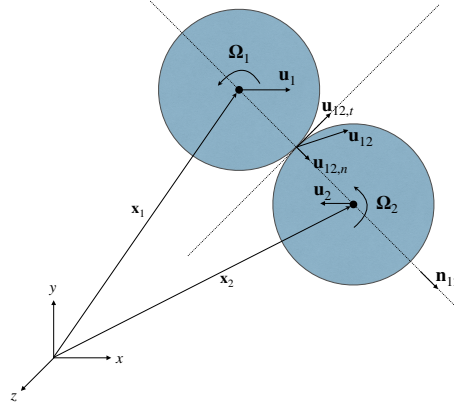


Figure A.1: Collision between two spherical particles: notations.

From Eqs. (A.1)-(A.4), it can be shown [19] that

$$\mathbf{u}'_{12} = \mathbf{u}_{12} + \frac{1}{m_{12}} \left(\left(1 + \frac{1}{K^2} \right) \mathbf{J} - \frac{1}{K^2} (\mathbf{J} \cdot \mathbf{n}_{12}) \mathbf{n}_{12} \right), \quad (\text{A.11})$$

where $m_{12} = \frac{m_1 m_2}{m_1 + m_2}$ is the reduced (or effective) mass and K is the normalized gyration radius. For as sphere, $K^2 = \frac{2}{5}$ so that Eq. (A.11) reads

$$\mathbf{u}'_{12} = \mathbf{u}_{12} + \frac{1}{2m_{12}} (7\mathbf{J} - 5(\mathbf{J} \cdot \mathbf{n}_{12})\mathbf{n}_{12}). \quad (\text{A.12})$$

To close the problem, Walton [150] proposed a simple hard-sphere model with three parameters (all between 0 and 1): a normal restitution coefficient e_n , a tangential restitution coefficient in the absence of sliding e_t and a friction coefficient μ_c to account for the transition between sticking and sliding regimes. According to Walton's model, the contact point pre- and post-collision velocities are linked by

$$\mathbf{n}_{12} \cdot \mathbf{u}'_{12} = -e_n(\mathbf{n}_{12} \cdot \mathbf{u}_{12}), \quad (\text{A.13})$$

$$\mathbf{n}_{12} \wedge \mathbf{u}'_{12} = -\beta(\mathbf{n}_{12} \wedge \mathbf{u}_{12}), \quad (\text{A.14})$$

where β ($-1 \leq \beta \leq 1$) is the general rotational restitution coefficient, which is equal to e_t in the absence of sliding. From Eqs. (A.12), (A.13) and (A.14), it is possible to obtain an expression for the normal and tangential components of the impulse vector:

$$\mathbf{J}_n = -(1 + e_n) m_{12}(\mathbf{u}_{12} \cdot \mathbf{n}_{12}), \quad (\text{A.15})$$

$$\mathbf{J}_t = -\left(\frac{K^2}{K^2 + 1}\right) (1 + \beta) m_{12}(\mathbf{u}_{12} \cdot \mathbf{t}_{12}), \quad (\text{A.16})$$

Eq. (A.16) is valid only when the contact is not sliding, i.e. when $|J_t| < \mu_c |J_n|$ according to Coulomb's friction law. This last condition is equivalent to

$$\frac{\|\mathbf{u}_{12,n}\|}{\|\mathbf{u}_{12,t}\|} > \left(\frac{K^2}{K^2 + 1}\right) \frac{(1 + \beta)}{\mu_c(1 + e_n)}. \quad (\text{A.17})$$

A general expression for the tangential impulse is then given by

$$\mathbf{J}_t = \begin{cases} \mathbf{J}_{t,0} = -\left(\frac{K^2}{K^2 + 1}\right) (1 + e_t) m_{12}(\mathbf{u}_{12} \cdot \mathbf{t}_{12}), & |J_{t,0}| < \mu_c |J_n|, \\ -\mu_c |J_n|, & |J_{t,0}| > \mu_c |J_n|. \end{cases} \quad (\text{A.18})$$

Walton formulated the above theory in terms of a general tangential restitution coefficient whose value is set according to the friction regime (sliding / sticking):

$$\beta = \begin{cases} \beta^* = -1 + \mu_c (1 + e_n) \left(1 + \frac{1}{K^2}\right) \frac{\|\mathbf{u}_{12,n}\|}{\|\mathbf{u}_{12,t}\|}, & \beta^* < e_t \text{ (sliding)}, \\ e_t, & \beta^* \geq e_t \text{ (sticking)}, \end{cases} \quad (\text{A.19})$$

This clipping of the rotational restitution coefficient when $\beta^* \geq e_t$ is illustrated in Figure A.2. With that formulation, the tangential impulse can always be expressed by Eq. (A.16), with the value of β determined by Eq. (A.19).

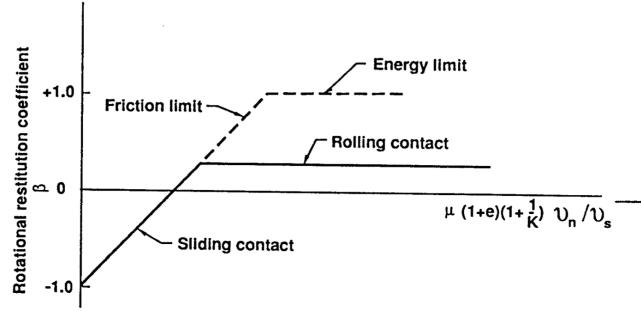


Figure A.2: General rotational restitution coefficient β in the sliding and sticking (or rolling) regimes. Reproduced from Walton [150], chapter 25, Fig. 25-7.

In the context of a hard-sphere model, it is common to define the incident and rebound angles, ϕ_{in} and ϕ_{out} as the angles formed by the collision normal vector and the contact point velocity before and after the collision, respectively (i.e. $\phi_i n = 0$ for a normal collision). It is however more convenient to work with the tangent of these angles, defined as

$$\Psi_{in} = \frac{\mathbf{u}_{12} \cdot \mathbf{t}_{12}}{\mathbf{u}_{12} \cdot \mathbf{n}_{12}} = \tan(\phi_{in}), \quad (\text{A.20})$$

$$\Psi_{out} = -\frac{\mathbf{u}'_{12} \cdot \mathbf{t}_{12}}{\mathbf{u}'_{12} \cdot \mathbf{n}_{12}} = \tan(\phi_{out}). \quad (\text{A.21})$$

According to Walton's model, the tangent of the rebound angle is given by

$$\Psi_{out} = -\frac{\beta}{e_n} \Psi_{in}, \quad (\text{A.22})$$

with β given by Eq. (A.19), which yields

$$\Psi_{out} = \begin{cases} -\frac{e_t}{e_n} \Psi_{in}, & \Psi_{in} < \Psi_{in}^* \text{ (sticking),} \\ \frac{1}{e_n} \Psi_{in} - \mu_c \left(1 + \frac{1}{e_n}\right) \left(1 + \frac{1}{K}\right), & \Psi_{in} > \Psi_{in}^* \text{ (sliding),} \end{cases} \quad (\text{A.23})$$

where Ψ_{in}^* is the tangent of the critical angle of incidence above which sliding occurs. The value of Ψ_{in}^* is obtained by imposing the continuity of Ψ_{out} at the friction regime transition:

$$\Psi_{out}(\Psi_{in}^{*+}) = \Psi_{out}(\Psi_{in}^{*-}) \Leftrightarrow \Psi_{in}^* = \mu_c \left(1 + \frac{1}{K}\right) \frac{(1 + e_n)}{(1 + e_t)}. \quad (\text{A.24})$$

A.2 Soft-sphere model

In our IBM, the particle-particle and particle-wall contacts are solved using a soft-sphere collision model derived from the original version proposed by Cundall and Strack [20]. We present two variants of this model: the one detailed by van der Hoef et al. in [144], which will be referred to as the standard model, and the most recent version of Costa et al. [18].

A.2.1 Standard model

In the soft-sphere model, particles are allowed to overlap over a short distance and the inter-particle contacts are represented using a spring-dashpot system in the normal and tangential directions, as sketched in Figs. A.3. A slider is added to represent Coulomb's friction limit. The conventions used to describe the contact between two particles are the same as given in Figure A.1.

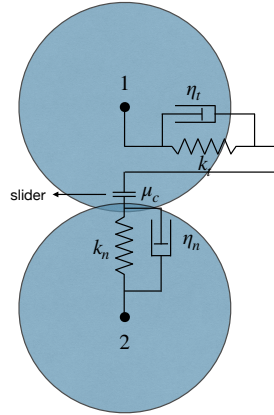


Figure A.3: Soft-sphere model: spring-dashpot system with a slider.

Considering that the effect of the spring element is linear (Hooke's law), the normal component of the contact force between the two bodies is expressed as

$$\mathbf{F}_{12,n} = -k_n \delta_{12,n} - \eta_n \mathbf{u}_{12,n}, \quad (\text{A.25})$$

where k_n and η_n are respectively the normal spring stiffness and damping coefficient and $\delta_{12,n}$ is the normal overlap vector, defined as

$$\delta_{12,n} = (R_1 + R_2 - \|\mathbf{x}_2 - \mathbf{x}_1\|)\mathbf{n}_{12}. \quad (\text{A.26})$$

The tangential component of the repulsion force is determined in a similar way, with an upper limit on its norm fixed by Coulomb's friction law (transition to sliding regime):

$$\mathbf{F}_{12,t} = \begin{cases} \mathbf{F}_{12,t}^0 = -k_t \delta_{12,t} - \eta_t \mathbf{u}_{12,t}, & \|\mathbf{F}_{12,t}^0\| \leq \mu_c \|\mathbf{F}_{12,n}\|, \\ -\mu_c \|\mathbf{F}_{12,n}\| \mathbf{t}_{12}, & \|\mathbf{F}_{12,t}^0\| > \mu_c \|\mathbf{F}_{12,n}\|, \end{cases} \quad (\text{A.27})$$

where k_t and η_t are the tangential stiffness and damping coefficient, respectively, and where the tangential unit vector $\mathbf{t}_{12}$ is defined by Eq. (A.10).

The tangential overlap $\delta_{12,t}$ is determined at each time step by adding the tangential displacement increment to the cumulative overlap. However, the previous tangential overlap vector $\delta_{12,t}^0$ must first be rotated in order to lie in the collision plane defined by the new normal vector. This rotation is defined by the vector $\mathbf{n}_{12} \wedge \mathbf{n}_{12,0}$, where $\mathbf{n}_{12,0}$ corresponds to the previous normal vector. In the absence of sliding, the tangential overlap is then calculated as

$$\delta_{12,t} = \delta_{12,t}^0 \cdot \mathbf{H} + \mathbf{u}_{12,t} \Delta t_s. \quad (\text{A.28})$$

The rotation matrix $\mathbf{H}$ is given by

$$\mathbf{H} = \begin{pmatrix} qh_x^2 + c & qh_x h_y - sh_z & qh_x h_z + sh_y \\ qh_x h_y + sh_z & qh_y^2 + c & qh_x h_z - sh_x \\ qh_x h_z - sh_y & qh_x h_z + sh_x & qh_z^2 + c \end{pmatrix}, \quad (\text{A.29})$$

where

$$\mathbf{h} = \frac{\mathbf{n}_{12} \wedge \mathbf{n}_{12,0}}{\|\mathbf{n}_{12} \wedge \mathbf{n}_{12,0}\|}, \quad c = \cos \phi, \quad s = \sin \phi, \quad q = 1 - c \quad \text{and} \quad \phi = \arcsin(\|\mathbf{n}_{12} \wedge \mathbf{n}_{12,0}\|). \quad (\text{A.30})$$

When sliding occurs, the tangential repulsion force becomes independent of δ_t . However, if the tangential overlap keeps being incremented in the sliding regime, unrealistic forces can be obtained if the friction regime transitions to sticking at some point during the contact. Therefore, Brendel and Dippel [12] proposed to set $\delta_t = \frac{\mu_c}{k_t} \|\mathbf{F}_{12,n}\| \mathbf{t}_{12}$ in the sliding regime, so that

$$\delta_{12,t} = \begin{cases} \delta_{12,t}^0 \cdot \mathbf{H} + \mathbf{u}_{12,t} \Delta t_s, & \|\mathbf{F}_{12,t}^0\| \leq \mu_c \|\mathbf{F}_{12,n}\|, \\ \frac{\mu_c}{k_t} \|\mathbf{F}_{12,n}\| \mathbf{t}_{12}, & \|\mathbf{F}_{12,t}^0\| > \mu_c \|\mathbf{F}_{12,n}\|. \end{cases} \quad (\text{A.31})$$

Finally, the force and torque acting on body 1 as a result of its contact with body 2 are given by

$$\mathbf{F}_{12,c} = \mathbf{F}_{12,t} + \mathbf{F}_{12,n}, \quad (\text{A.32})$$

and

$$\mathbf{M}_{12,c} = R_1(\mathbf{n}_{12} \wedge \mathbf{F}_{12,c}). \quad (\text{A.33})$$

The total collision force and torque acting on a particle i is obtained by summing the contributions of all contacting particles, i.e.

$$\mathbf{F}_{i,c} = \sum_j \mathbf{F}_{ij,c}, \quad (\text{A.34})$$

$$\mathbf{M}_{i,c} = \sum_j \mathbf{M}_{ij,c}. \quad (\text{A.35})$$

Hence, a major advantage of the soft-sphere model lies in its ability to handle non-binary collisions that can be observed in dense particle flows.

For particle-wall collisions, we consider that the wall acts as a particle with zero velocity, infinite radius and infinite mass (i.e. $m_2, R_2 \rightarrow \infty$) and the particle-wall normal overlap is computed as

$$\delta_n = (R_1 - d_{\text{wall}})\mathbf{n}_w, \quad (\text{A.36})$$

with $\mathbf{n}_w$, the unit normal vector pointing into the wall and d_{wall} , the distance between the wall and the center of the particle.

A.2.2 Costa's variant

In [18], Costa et al. propose a variant of the standard model concerning the tangential component of the repulsion force. Eq (A.27) is modified as

$$\mathbf{F}_{12,t} = \begin{cases} \mathbf{F}_{12,t}^0 = -k_t \delta_{12,t} - \eta_t \mathbf{u}_{12,t}, & \|\mathbf{F}_{12,t}^0\| \leq \mu_c \|\mathbf{F}_{12,n}\|, \\ \mu_c \|\mathbf{F}_{12,n}\| \mathbf{t}_{12}, & \|\mathbf{F}_{12,t}^0\| > \mu_c \|\mathbf{F}_{12,n}\|, \end{cases} \quad (\text{A.37})$$

where the tangential vector is now defined as

$$\mathbf{t}_{12} = \frac{\mathbf{F}_{12,t}^0}{\|\mathbf{F}_{12,t}^0\|}. \quad (\text{A.38})$$

In other words, $\mathbf{t}_{12}$ is no longer aligned with the tangential component of the contact point velocity but with the "test force" $\mathbf{F}_{12,t}^0$. In 2-D, this will just result in a change of

sign, but in 3-D, $\mathbf{F}_{12,t}^0$ and $\mathbf{u}_{12,t}$ might not be aligned although they both belong to the plane orthogonal to the normal vector $\mathbf{n}_{12}$.

Moreover, Costa et al. [18] fix the value of δ_t in the sliding regime in order to ensure the continuity of the tangential repulsion force when transition occurs between the sliding and the non-sliding regimes. The general expression of the tangential overlap is now given by

$$\delta_{12,t} = \begin{cases} \delta_{12,t}^0 \cdot \mathbf{H} + \mathbf{u}_{12,t} \Delta t_s, & \|\mathbf{F}_{12,t}^0\| \leq \mu_c \|\mathbf{F}_{12,n}\|, \\ \frac{1}{k_t} (-\mu_c \|\mathbf{F}_{12,n}\| \mathbf{t}_{12} - \eta_t \mathbf{u}_{12,t}), & \|\mathbf{F}_{12,t}^0\| > \mu_c \|\mathbf{F}_{12,n}\|. \end{cases} \quad (\text{A.39})$$

Our own implementation of the soft-sphere model is based on Costa's variant as supported by the thorough collision study in Section 1.5.5.

A.2.3 Model parameters

To solve the model described by Eqs. (A.25) and (A.27), we need to specify five parameters: k_n , η_n , k_t , η_t and μ_c . The damping coefficients η_n and η_t can be obtained from the stiffness values and the restitution coefficients e_n and e_t . Along the normal direction, η_n is given by

$$\eta_n = \begin{cases} -\frac{2 \log e_n}{\sqrt{\pi^2 + \log^2(e_n)}} \sqrt{m_{12} k_n}, & e_n \neq 0, \\ 2 \sqrt{m_{12} k_n}, & e_n = 0, \end{cases} \quad (\text{A.40})$$

with the reduced mass $m_{12} = \frac{m_1 m_2}{m_1 + m_2}$. Similarly along the tangential direction, we have that

$$\eta_t = \begin{cases} -\frac{2 \log e_t}{\sqrt{\pi^2 + \log^2(e_t)}} \sqrt{m'_{12} k_t}, & e_t \neq 0, \\ 2 \sqrt{m'_{12} k_t}, & e_t = 0, \end{cases} \quad (\text{A.41})$$

with $m'_{12} = \frac{2}{7} m_{12}$ for a sphere.

The values of the stiffnesses k_n and k_t can be obtained theoretically from the Hertzian theory when the material properties of the solid (Young modulus, Poisson ratio) are known [62]. However, the resulting values lead to impractically small time steps and, in practice, their values must be chosen smaller. Typically, we will fix the value of the stiffness such that the duration of a collision spans over at least 10 fluid time steps. If the maximum overlap happens to be unphysically large ($> 1\%$ of the

characteristic size of the body), we must reduce the time step to make the collision "stiffer". Using the harmonic oscillator theory, the collision contact time can be expressed as (see [144]):

$$T_n = \sqrt{\frac{\pi^2 + (\log(e_n))^2}{k_n/m_{12}}}. \quad (\text{A.42})$$

If K_N is the number of fluid time steps used to resolve a collision and assuming that $e_n = e_t$, we have that

$$\Delta t = \frac{1}{K_N} T_n = \frac{1}{K_N} \sqrt{\frac{\pi^2 + (\log(e_n))^2}{k_n/m_{12}}} = \frac{1}{K_N} \sqrt{\frac{\pi^2 + (\log(e_t))^2}{k_t/m'_{12}}}. \quad (\text{A.43})$$

By fixing K_N , Eq. (A.43) allows the computation of the stiffnesses for a given fluid time step as

$$k_n = \frac{m_{12}(\pi^2 + (\log(e_n))^2)}{(K_N \Delta t)^2} \quad (\text{A.44})$$

and

$$k_t = \frac{m'_{12}(\pi^2 + (\log(e_t))^2)}{(K_N \Delta t)^2}. \quad (\text{A.45})$$

It must be noted that the collision time T_n is chosen as a multiple of the fluid time step, so that the fluid can adapt to rapid changes in particle velocity. Based on the discussion in [18], we use $K_N = 10$ in this work.

A.3 Lubrication

Hydrodynamic stresses resulting from the approach of two bodies (or a body and a wall) can be captured on the cartesian grid with the IBM until the gap width becomes smaller than the grid size. After that, it can be expected that the short-range hydrodynamic forces will be largely underestimated by the IBM. Therefore, several authors [22, 11, 145, 18] have proposed to add a lubrication correction force in the equations of motion based on analytical solutions available for canonical lubrication interactions (e.g. sphere-sphere, sphere-plane) in the Stokes regime. In this work, we only consider the addition of lubrication forces along the normal direction as supported by the exhaustive study in [14]. More specifically, we consider the three-layer lubrication model proposed in the same study and illustrated in Figure A.4

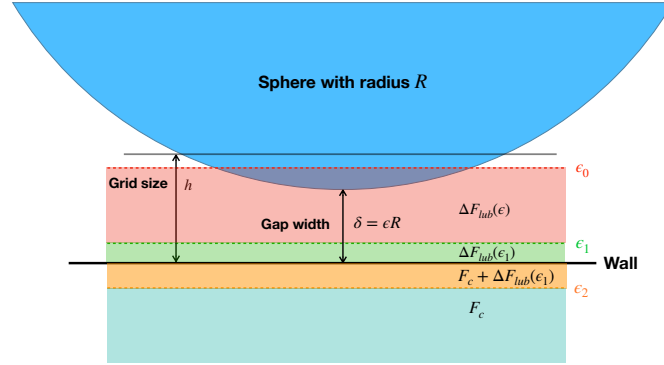


Figure A.4: Combined soft-sphere lubrication model. Illustration inspired from [14] for a sphere approaching a wall.

One defines the non-dimensional gap width $\epsilon = \delta/R$, where δ is here the signed distance between the two particles or between the particle and the wall (positive before contact, negative after contact¹). Considering that the IBM no longer captures the fluid forces below a certain gap width ϵ_0 , the lubrication force correction is taken as

$$\Delta \mathbf{F}_{lub} = -6\pi R \mathbf{u}_{12,n} (\lambda(\epsilon) - \lambda(\epsilon_0)), \quad (\text{A.46})$$

where λ is the Stokes amplification factor. It is expressed as [60]²

$$\lambda_{pp}(\epsilon) = \frac{1}{4\epsilon} - \frac{9}{40} \log \epsilon - \frac{3}{112} \epsilon \log \epsilon + \mathcal{O}(1) \quad (\text{A.47})$$

for two approaching spheres and as

$$\lambda_{pw}(\epsilon) = \frac{1}{\epsilon} - \frac{1}{5} \log \epsilon - \frac{1}{21} \epsilon \log \epsilon + \mathcal{O}(1) \quad (\text{A.48})$$

for a sphere approaching a wall.

¹Pay attention that this sign convention is opposite to that used in the definition of the normal overlap in the soft-sphere model (Eq. (A.26))

²Note that there is a factor 2 between the expression reported for λ_{pp} in [60] and Eq. (A.47) as we chose to express the lubrication force as a function of the *relative* normal velocity $\mathbf{u}_{12,n}$ instead of the less general *incident* velocity formulation

The expression for $\Delta \mathbf{F}_{lub}$ in Eq. (A.46) diverges for a vanishing gap. To account for surface roughness, the Stokes amplification factor is saturated when the gap width ϵ goes below a given threshold ϵ_1 , so that $\lambda(\epsilon < \epsilon_1) = \lambda(\epsilon_1)$. Also, to ensure a smooth transition between the lubrication and the contact forces, the lubrication correction is preserved after the contact up to a (small) negative overlap $-\epsilon_2$, as proposed in [14]. Finally, the lubrication force acting on the particle is computed as

$$\frac{\Delta \mathbf{F}_{lub}}{-6\pi\mu R \mathbf{u}_{12n}} = \begin{cases} \lambda(\epsilon) - \lambda(\epsilon_0), & \epsilon_1 \leq \epsilon < \epsilon_0 \\ \lambda(\epsilon_1) - \lambda(\epsilon_0), & -\epsilon_2 \leq \epsilon < \epsilon_1 \\ 0, & \text{otherwise.} \end{cases} \quad (\text{A.49})$$

The values given to the parameters ϵ_0 , ϵ_1 and ϵ_2 are discussed in our validation procedure (Section 1.5.4).

Momentum balance and drag force definitions

We clarify here the link between the different formulations of the mean drag force and the pressure gradient acting on a fluid-particle system. The developments below are partly inspired from [143].

We consider the flow of a fluid at constant superficial (i.e. flow rate) velocity $\mathbf{U}_0 = U_0 \mathbf{e}_\parallel$ through a fixed assembly of particles with solid volume fraction ϕ_s . The fluid-phase averaged (or interstitial) velocity is $\mathbf{u}_f = \mathbf{U}_0/(1 - \phi_s)$. The particle Reynolds number is given by $\text{Re}_p = \frac{\rho_f d_p U_0}{\mu}$. Since the fluid flows at constant velocity, the pressure drop across the domain of volume V must compensate the total force exerted by the N_p particles included in this volume, which reads

$$-V \nabla p = N_p \mathbf{F}_p, \quad (\text{B.1})$$

where $\mathbf{F}_p$ corresponds to the total average force that the fluid exerts on each particle. The latter can be decomposed as

$$\mathbf{F}_p = \mathbf{F}_d - V_p \nabla p, \quad (\text{B.2})$$

where $\mathbf{F}_d$ is the drag term, i.e. the friction induced by the fluid at the surface of the particle as soon as their relative velocity is non-zero. The second term is a buoyancy-type term due to pressure gradient ∇p applied over the volume V_p of the particle. Since $\phi_s = \frac{N_p V_p}{V}$, the combination of (B.1) and (B.2) gives

$$\mathbf{F}_d = -\frac{(1 - \phi_s)}{\phi_s} V_p \nabla p \quad (\text{B.3})$$

and consequently,

$$\mathbf{F}_p = \frac{\mathbf{F}_d}{(1 - \phi_s)}, \quad (\text{B.4})$$

i.e. $\mathbf{F}_d$ and $\mathbf{F}_p$ coincide in the infinitely dilute regime. In the Stokes regime, the drag force experienced by a sphere in an unbounded domain is given by $3\pi\mu d_p \mathbf{U}_0$. It is therefore common to define the normalized drag force as

$$\bar{F}_d = \frac{\mathbf{F}_d \cdot \mathbf{e}_{\parallel}}{3\pi\mu d_p U_0}, \quad (\text{B.5})$$

so that $\bar{F}_d = 1$ when ϕ_s and Re_p tend to zero. By analogy, we also define the normalized total fluid-particle force as

$$\bar{F}_p = \frac{\mathbf{F}_p \cdot \mathbf{e}_{\parallel}}{3\pi\mu d_p U_0} = \frac{\bar{F}_d}{(1 - \phi_s)}. \quad (\text{B.6})$$

This quantity is more generally noted $\bar{F}$ in the rest of this thesis.

Another way of formulating the drag force is the drag coefficient C_d , defined as

$$C_d = \frac{\mathbf{F}_d}{\frac{1}{2}\rho_f U_0^2 A_p} \quad (\text{B.7})$$

where $A_p = \pi \frac{d_p^2}{4}$ is the projected surface for a sphere. Hence C_d and $\bar{F}_d$ are related by

$$C_d = \frac{24}{\text{Re}_p} \bar{F}_d. \quad (\text{B.8})$$

Finally, in chemical engineering and in a multiphase approach, the drag force is usually expressed in terms of a friction coefficient β , such that

$$-(1 - \phi_s)\nabla p = \beta(\mathbf{u}_f - \mathbf{u}_s) = \beta \mathbf{U}_0 / (1 - \phi_s), \quad (\text{B.9})$$

where $\mathbf{u}_s = 0$ for a fixed array of spheres, or, more generally, for any system studied in a reference frame moving at mean solid phase mean velocity. By taking the streamwise component of Eq. (B.9), and using Eqs. (B.3) and (B.5), the friction coefficient β can be expressed as

$$\beta = 18(1 - \phi_s)\phi_s \frac{\mu}{d_p^2} \bar{F}_d. \quad (\text{B.10})$$

Table B.1 summarizes the different expressions of the drag force and their values in the Stokes regime at infinite dilution.

	Relation to $\bar{F}_d$	Value in the Stokes regime at infinite dilution
$\bar{F}_d$	-	1
$\bar{F}_p$	$\frac{\bar{F}_d}{(1 - \phi_s)}$	1
C_d	$\frac{24}{\text{Re}_p} \bar{F}_d$	$\frac{24}{\text{Re}_p}$
β	$18(1 - \phi_s)\phi_s \frac{\mu}{d_p^2} \bar{F}_d$	0

Table B.1: Different formulations of the drag force in fluid-particle systems.

Derivation of the energy equation in the Euler-Euler model

The conservation equations of the Euler-Euler model are either postulated from the mixture theory ([7]) or derived from the averaging of the governing equations of the micro-scale flow [5, 29]. We reproduce here the derivation of the Euler-Euler energy equation using a volume averaging procedure as detailed in [136]. In a two-phase system, the conservative form of the energy equation in the the fluid phase reads

$$\frac{\partial}{\partial t} (\rho_f c_{p,f} T) + \nabla \cdot (\rho_f c_{p,f} \mathbf{u} T) = \nabla \cdot (k_f \nabla T). \quad (\text{C.1})$$

We multiply Eq. (C.1) by the fluid phase indicator function χ_f , and integrate over a control volume V , which yields

$$\int_V \chi_f \frac{\partial}{\partial t} (\rho_f c_{p,f} T) dV + \int_V \chi_f \nabla \cdot (\rho_f c_{p,f} \mathbf{u} T) dV = \int_V \chi_f \nabla \cdot (k_f \nabla T) dV. \quad (\text{C.2})$$

Using derivation rules, Eq. (C.2) can be re-arranged as

$$\begin{aligned} \int_V \left(\frac{\partial}{\partial t} (\chi_f \rho_f c_{p,f} T) - \rho_f c_{p,f} T \frac{\partial \chi_f}{\partial t} \right) dV + \int_V (\nabla \cdot (\chi_f \rho_f c_{p,f} \mathbf{u} T) - \rho_f c_{p,f} T \mathbf{u} \cdot \nabla \chi_f) dV \\ = \int_V \nabla \cdot (\chi_f k_f \nabla T) - k_f \nabla T \cdot \nabla \chi_f dV \end{aligned} \quad (\text{C.3})$$

and

$$\begin{aligned} \int_V \frac{\partial}{\partial t} (\chi_f \rho_f c_{p,f} T) dV - \int_V \rho_f c_{p,f} T \underbrace{\left(\frac{\partial \chi_f}{\partial t} + \mathbf{u} \cdot \nabla \chi_f \right)}_{= \frac{D\chi_f}{Dt}} dV + \int_V \nabla \cdot (\chi_f \rho_f c_{p,f} \mathbf{u} T) dV \\ = \int_V \nabla \cdot (\chi_f k_f \nabla T) dV - \int_V k_f \nabla T \cdot \nabla \chi_f dV. \quad (\text{C.4}) \end{aligned}$$

The phase indicator function obeys the transport equation

$$\frac{D\chi_f}{Dt} = \frac{\partial \chi_f}{\partial t} + \mathbf{u} \cdot \nabla \chi_f = 0 \quad (\text{C.5})$$

so that the second term in the left-hand side (lhs) of Eq. (C.4) vanishes. The gradient of the fluid phase indicator function is zero, except at the fluid-solid interface where it is aligned with the local normal vector, which yields

$$\nabla \chi_f(\mathbf{x}) = \mathbf{n}^f \delta_I(\mathbf{x} - \mathbf{x}_I), \quad (\text{C.6})$$

where $\mathbf{n}^f$ is the unit normal vector of the fluid-solid interface pointing towards the fluid phase and $\delta_I(\mathbf{x} - \mathbf{x}_I)$ is the Dirac delta function centered at the fluid-solid interface identified by the position vector $\mathbf{x}_I$. It follows that the second term in the right-hand side (rhs) of Eq. (C.4) gives the total heat flux transferred from the solid to the fluid phase in the volume V :

$$\mathcal{Q}_{s \rightarrow f} = - \int_V k_f \nabla T \cdot \nabla \chi_f dV = - \oint_{\partial V_s} k_f \nabla T \cdot \mathbf{n}^f dS \quad (\text{C.7})$$

where ∂V_s is the fluid-solid interface contained in the volume V . Then, Eq. (C.4) simplifies as

$$\int_V \frac{\partial}{\partial t} (\chi_f \rho_f c_{p,f} T) dV + \int_V \nabla \cdot (\chi_f \rho_f c_{p,f} \mathbf{u} T) dV = \int_V \nabla \cdot (\chi_f k_f \nabla T) dV + \mathcal{Q}_{s \rightarrow f}. \quad (\text{C.8})$$

Eq. (C.8) expresses the global heat balance over the control volume. At steady-state, the total heat flux transferred from the solid to the fluid phase can then be expressed as

$$\mathcal{Q}_{s \rightarrow f} = \int_V \nabla \cdot (\chi_f \rho_f c_{p,f} \mathbf{u} T) dV - \int_V \nabla \cdot (\chi_f k_f \nabla T) dV \quad (\text{C.9})$$

$$= \int_{\partial V} \chi_f \rho_f c_{p,f} (\mathbf{u} T) \cdot \mathbf{n} dS - \int_{\partial V} \chi_f k_f \nabla T \cdot \mathbf{n} dS, \quad (\text{C.10})$$

where $\mathbf{n}$ is the outwards unit normal vector on boundaries ∂V of the control volume.

We divide Eq. (C.8) by the control volume V and, assuming constant physical properties, the local energy equation of the macro-scale flow reads

$$\frac{\partial}{\partial t} (\rho_f c_{p,f} \phi_f \langle T^{(f)} \rangle) + \nabla \cdot (\rho_f c_{p,f} \phi_f \langle (\mathbf{u} T)^{(f)} \rangle) = \nabla \cdot (k_f \phi_f \nabla \langle T^{(f)} \rangle) + q_{s \rightarrow f}. \quad (\text{C.11})$$

where $q_{s \rightarrow f} = Q_{s \rightarrow f}/V$ is the heat flux exchange between the solid and the fluid phases per unit volume. In Eq. (C.11), we introduced the fluid-phase average operator $\langle \cdot \rangle^{(f)}$, defined for a given quantity ψ as

$$\langle \psi^{(f)} \rangle = \frac{1}{V_f} \int_{V_f} \psi(\mathbf{x}) \, dV = \frac{\int_V \chi_f(\mathbf{x}) \psi(\mathbf{x}) \, dV}{\int_V \chi_f(\mathbf{x}) \, dV}. \quad (\text{C.12})$$

and the local fluctuation of ψ is defined as

$$\psi'(\mathbf{x}) = \psi(\mathbf{x}) - \langle \psi^{(f)} \rangle. \quad (\text{C.13})$$

Then, using the following property,

$$\langle (\mathbf{u} T)^{(f)} \rangle = \langle \mathbf{u}^{(f)} \rangle \langle T^{(f)} \rangle + \langle (\mathbf{u}' T')^{(f)} \rangle, \quad (\text{C.14})$$

the second term on the left-hand side of Eq. (C.11) is split into a mean flow convective term and a term involving the correlation between the temperature and the velocity fields. Finally, Eq. (C.11) takes the form

$$\begin{aligned} & \frac{\partial}{\partial t} (\rho_f c_{p,f} \phi_f \langle T^{(f)} \rangle) + \nabla \cdot (\rho_f c_{p,f} \phi_f \langle \mathbf{u}^{(f)} \rangle \langle T^{(f)} \rangle) \\ &= \nabla \cdot (k_f \phi_f \nabla \langle T^{(f)} \rangle) + q_{s \rightarrow f} - \nabla \cdot (\rho_f c_{p,f} \phi_f \langle (\mathbf{u}' T')^{(f)} \rangle). \end{aligned} \quad (\text{C.15})$$

Particle self-diffusion and auto-correlation function

The theoretical analysis of fluid particles dispersion goes back to the pioneering works of Taylor [129] and Batchelor [8]. Investigations on the diffusion properties of heavy particles have been later carried out by Pismen et al. [99]. We reproduce here a derivation similar to that proposed by Mazzitelli et al. [82] to link the mean square displacement of solid particles to the particle velocity auto-correlation function.

The mean square displacement (MSD) tensor is defined as

$$M_{ij}(t) = \langle (x_{p,i}(t) - x_{p,i}(t_0))(x_{p,j}(t) - x_{p,j}(t_0)) \rangle \quad (\text{D.1})$$

where t_0 is the initial observation time. In the absence of collective motion, the displacement of a particle after a time t is expressed as

$$x_{p,i}(t) = x_{p,i}(t_0) + \int_{t_0}^t u'_{p,i}(t') dt'. \quad (\text{D.2})$$

Hence, the diagonal components of the MSD tensor can be expressed as

$$M_{ii}(t) = \left\langle \int_{t_0}^t dt' \int_{t_0}^t dt'' u'_{p,i}(t') u'_{p,i}(t'') \right\rangle, \quad (\text{D.3})$$

where $i = x, y$ or z (no summation on the repeated index). When the flow has reached a statistical steady state, the integral and averaging operator can commute, so that

$$M_{ii}(t) = \int_{t_0}^t dt' \int_{t_0}^t dt'' \langle u'_{p,i}(t') u'_{p,i}(t'') \rangle. \quad (\text{D.4})$$

It can also be observed that the integration area is a square. Since the bi-variate function $\langle u'_{p,i}(t')u'_{p,i}(t'') \rangle$ takes identical values on both sides of the line $t' = t''$, the bounds of the inner integral can be modified to give

$$M_{ii}(t) = 2 \int_{t_0}^t dt' \int_{t_0}^{t'} dt'' \langle u'_{p,i}(t')u'_{p,i}(t'') \rangle. \quad (\text{D.5})$$

Using the change of variable $\tau = t'' - t'$, Eq. (D.5) is recast as

$$M_{ii}(t) = 2 \int_{t_0}^t dt' \int_{-(t'-t_0)}^0 d\tau \langle u'_{p,i}(t')u'_{p,i}(t' + \tau) \rangle. \quad (\text{D.6})$$

The particle velocity auto-correlation function is defined as

$$R_{U_i U_i}(\tau) = \frac{\langle u'_{p,i}(t)u'_{p,i}(t + \tau) \rangle}{\langle u'^2_{p,i}(t) \rangle}. \quad (\text{D.7})$$

Since $R_{U_i U_i}(\tau)$ is even, i.e. symmetric under the transformation $\tau \rightarrow -\tau$, we have that

$$M_{ii}(t) = 2 \langle u'^2_{p,i} \rangle \int_{t_0}^t dt' \int_0^{t'-t_0} d\tau R_{U_i U_i}(\tau). \quad (\text{D.8})$$

We now analyse the asymptotic behavior of M_{ii} . For short separation times, $R_{U_i U_i}(\tau) \simeq 1$, which gives

$$M_{ii}(t) \simeq 2 \langle u'^2_{p,i} \rangle \int_{t_0}^t dt' (t' - t_0) = \langle u'^2_{p,i} \rangle (t - t_0)^2. \quad (\text{D.9})$$

For large separation times we have that

$$\int_0^{t'-t_0} d\tau R_{U_i U_i}(\tau) \simeq \int_0^\infty d\tau R_{U_i U_i}(\tau) = \mathcal{T}_{U_i}, \quad (\text{D.10})$$

where $\mathcal{T}_{U_i}$ is the particle velocity Lagrangian time scale. In that case, M_{ii} can be expressed as

$$M_{ii}(t) \simeq 2 \langle u'^2_{p,i} \rangle \mathcal{T}_{U_i} (t - t_0). \quad (\text{D.11})$$

Finally, the diffusion coefficient $\mathcal{D}_i$ in direction $i = x, y, z$ is obtained as

$$\mathcal{D}_i = \lim_{t \rightarrow \infty} \frac{1}{2} \frac{d}{dt} M_{ii}(t) = \langle u'^2_{p,i} \rangle \mathcal{T}_{U_i}. \quad (\text{D.12})$$

A sharp interface method for scalar fields in 2-D

In Chapter 1, the IBM was developed to impose Dirichlet conditions on the scalar fields and ensure their continuity at the surface of the particles. The temperature of the particle was taken constant in time (i.e. infinite heat capacity assumption) or free to evolve as the result of the balance between heat source terms and interfacial fluxes (see Eq. (1.10)). In both cases, T_p was considered spatially uniform in the particle. Actually, this assumption is fairly well verified for particles characterized by a small Biot number $Bi = \frac{h_f d_p}{k_s}$ where h_f is the heat transfer coefficient between the fluid and the particle. This is for example the case of the small catalytic particles used in fluid catalytic cracking (FCC) where $Bi \sim \mathcal{O}(10^3)$. Species concentration gradients are however more prone to appear as the ratio of mass diffusivities between the solid and the fluid phase is typically smaller than the thermal conductivity ratio. Therefore, there may be situations where it is of interest to solve the heat and/or mass transfer problem in the solid phase. In that case, the IBM is no longer used for the scalar fields. Instead, the governing equations for the temperature and/or concentration fields are modified according to the location of each phase. The discontinuity that appears at the surface of the particle can be either captured in a diffuse way using only the phase indicator function, or in a sharp way by keeping the details about the exact location of the interface.

In this appendix, we present a sharp interface (SI) method based on the original method proposed by Liu et al. [74] to solve the Poisson equation on irregular domains. It was later combined to the DLM/FD method and applied to heat and mass transfer by Shao et al. [111] and Sulaiman et al. [119]. We first describe the salient features of

the method. Then, the method is validated from analytical results and its accuracy is evaluated by comparison to the diffuse interface (DI) method.

E.1 Modified governing equations

The governing equations for the temperature and concentration fields in the entire domain are now given by

$$\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T = \frac{1}{\tilde{\rho}\tilde{c}_p} \nabla \cdot (\tilde{k} \nabla T) + \tilde{S}_T \quad (\text{E.1})$$

and

$$\frac{\partial C_\alpha}{\partial t} + \mathbf{u} \cdot \nabla C_\alpha = \nabla \cdot (\tilde{D}_\alpha \nabla C_\alpha) + \tilde{S}_\alpha \quad (\text{E.2})$$

where the value taken by a ‘~’ quantity depends on the phase indicator function. More specifically, for any quantity ψ , we have that

$$\tilde{\psi}(\mathbf{x}, t) = (1 - \chi_s(\mathbf{x}, t))\psi_f + \chi_s(\mathbf{x}, t)\psi_s, \quad (\text{E.3})$$

where ‘ f ’ and ‘ s ’ subscripts represent the fluid and solid phase values, respectively¹. At the fluid/solid interface Γ , the scalar fields and the heat and mass fluxes must be continuous, which reads

$$[T]_\Gamma = [C_\alpha]_\Gamma = 0, \quad (\text{E.4})$$

$$\left[\tilde{k} \frac{\partial T}{\partial n} \right]_\Gamma = \left[\tilde{D}_\alpha \frac{\partial C_\alpha}{\partial n} \right]_\Gamma = 0. \quad (\text{E.5})$$

where $[\]_\Gamma$ is the jump operator across the interface.

In the DI method, Eqs. (E.2) and (E.1) are solved without modifying the spatial discretization of the differential operators and the transport coefficients that must be evaluated at the faces of the grid cells are simply obtained as the average of the cell-centered values, e.g. $\tilde{D}_{\alpha,i+1/2} = \frac{1}{2} (\tilde{D}_{\alpha,i} + \tilde{D}_{\alpha,i+1})$ whether there is an interface between i and $i + 1$ or not. The SI method presented here is used to discretize the diffusion term while the convection term is kept unchanged as it is expected to be less dominant close to the interface. We first illustrate the SI method in the one-dimensional case and then discuss the particular features that appear in two dimensions. It must also be noted that the present SI method is first-order in space close to the interface, as shown by the convergence studies in [74].

¹Regarding density, the reference value in the fluid is ρ_{f0}

E.2 Sharp interface method in one dimension

Let us first consider the one-dimensional diffusion term $\frac{\partial}{\partial x} \left(\beta \frac{\partial f}{\partial x} \right)$ for a given quantity f (temperature or concentration) with transport coefficient β . When an interface Γ is introduced between the grid points i and $i+1$, the domain is split into two sub-domains Ω^- and Ω^+ as shown in Figure E.1 and the grid cell crossed by the interface is divided into two sub-cells of widths θh on the left and $(1-\theta)h$ on the right. General jump conditions are provided at the interface:

$$a_\Gamma \triangleq [f]_\Gamma = f^+ - f^- \quad (\text{E.6})$$

$$b_\Gamma \triangleq \left[\beta \frac{\partial f}{\partial x} \right]_\Gamma = \left(\beta \frac{\partial f}{\partial x} \right)_\Gamma^+ - \left(\beta \frac{\partial f}{\partial x} \right)_\Gamma^-, \quad (\text{E.7})$$

where '+' and '-' superscripts indicate the evaluation of the quantity on each side of Γ .

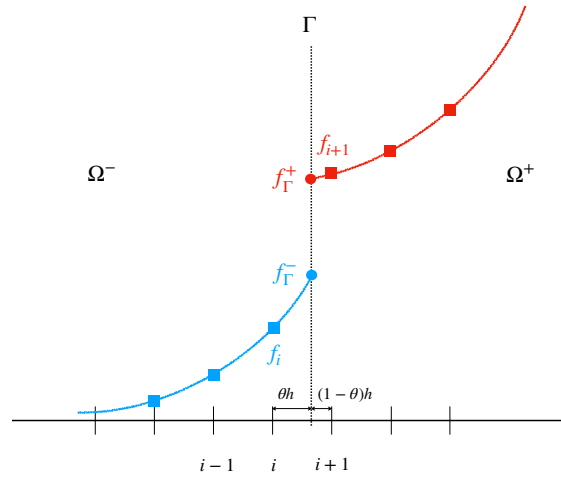


Figure E.1: Schematic 1-D plot of the discontinuities of a function f (and its derivatives) created by the introduction of an interface Γ between two grid points.

Away from the interface, the 1-D diffusion operator at a grid point k can be discretized with classical second order centered finite differences:

$$\frac{\partial}{\partial x} \left(\beta \frac{\partial f}{\partial x} \right) \Big|_k = \frac{1}{h} \left(\beta_{k+1/2} \frac{f_{k+1} - f_k}{h} - \beta_{k-1/2} \frac{f_k - f_{k-1}}{h} \right). \quad (\text{E.8})$$

At grid points i and $i + 1$, Eq. (E.8) must be modified to account for the discontinuities created by the interface, i.e.

$$\left. \frac{\partial}{\partial x} \left(\beta \frac{\partial f}{\partial x} \right) \right|_i = \frac{1}{h} \left(\beta^- \left(\frac{f_\Gamma^- - f_i}{\theta h} \right) - \beta^- \left(\frac{f_i - f_{i-1}}{h} \right) \right) \quad (\text{E.9})$$

$$\left. \frac{\partial}{\partial x} \left(\beta \frac{\partial f}{\partial x} \right) \right|_{i+1} = \frac{1}{h} \left(\beta^+ \left(\frac{f_{i+2} - f_{i+1}}{h} \right) - \beta^+ \left(\frac{f_{i+1} - f_\Gamma^+}{(1-\theta)h} \right) \right), \quad (\text{E.10})$$

where the values of f on each side of the interface are unknown. The jump condition b_Γ can be discretized as

$$\begin{aligned} b_\Gamma &= \beta^+ \left(\frac{f_{i+1} - f_\Gamma^+}{(1-\theta)h} \right) - \beta^- \left(\frac{f_\Gamma^- - f_i}{\theta h} \right) \\ &= \beta^+ \left(\frac{f_{i+1} - (f_\Gamma^- + a_\Gamma)}{(1-\theta)h} \right) - \beta^- \left(\frac{f_\Gamma^- - f_i}{\theta h} \right) \end{aligned} \quad (\text{E.11})$$

and f_Γ^- is then given by

$$f_\Gamma^- = \frac{\theta \beta^+ (f_{i+1} - a_\Gamma) + (1-\theta) \beta^- f_i - (1-\theta) \theta h b_\Gamma}{\theta \beta^+ + (1-\theta) \beta^-}. \quad (\text{E.12})$$

Introducing Eq. (E.12) into Eq. (E.9) yields the following expression for the diffusion term at grid point i ,

$$\left. \frac{\partial}{\partial x} \left(\beta \frac{\partial f}{\partial x} \right) \right|_i = \frac{1}{h} \left(\hat{\beta} \left(\frac{f_{i+1} - f_i}{h} \right) - \beta^- \left(\frac{f_i - f_{i-1}}{h} \right) \right) - \frac{\hat{\beta} a_\Gamma}{h^2} - \frac{\hat{\beta} (1-\theta) b_\Gamma}{\beta^+ h}, \quad (\text{E.13})$$

where $\hat{\beta}$ is defined as

$$\hat{\beta} = \frac{\beta^+ \beta^-}{\theta \beta^+ + \beta^- (1-\theta)}. \quad (\text{E.14})$$

In the same way, the diffusion term at grid point $i + 1$ is expressed as

$$\left. \frac{\partial}{\partial x} \left(\beta \frac{\partial f}{\partial x} \right) \right|_{i+1} = \frac{1}{h} \left(\beta^+ \left(\frac{f_{i+2} - f_{i+1}}{h} \right) - \hat{\beta} \left(\frac{f_{i+1} - f_i}{h} \right) \right) + \frac{\hat{\beta} a_\Gamma}{h^2} - \frac{\hat{\beta} \theta b_\Gamma}{\beta^- h}. \quad (\text{E.15})$$

When both the scalar function f and the flux $\beta \frac{\partial f}{\partial x}$ are continuous at the interface we have $a_\Gamma = 0$ and $b_\Gamma = 0$, so that the expressions (E.13) and (E.15) simplify drastically.

E.3 Extension to two dimensions

We now consider the diffusion operator $\nabla \cdot (\beta \nabla f)$ in two dimensions with the following jump conditions at the interface:

$$a_\Gamma = [f]_\Gamma = 0 \quad (\text{E.16})$$

$$b_\Gamma = \left[\beta \frac{\partial f}{\partial n} \right]_\Gamma = 0. \quad (\text{E.17})$$

The unit normal $\mathbf{n} = (n_x, n_y)$ is defined by

$$\mathbf{n} = \frac{\nabla \phi}{|\nabla \phi|}, \quad (\text{E.18})$$

with ϕ , the level set function, i.e. the signed distance to the closest interface point. As a convention, $\phi \leq 0$ in Ω^- and $\phi > 0$ in Ω^+ . Hence, $\mathbf{n}$ points from Ω^- to Ω^+ as shown in Figure E.2. It must be noted that the jump condition b_Γ is now given in terms of the derivative normal to the interface while nothing is specified along the tangential direction $\mathbf{s}$. Applying the approach developed in one dimension along each cartesian direction, the 2-D diffusion term has the general expression

$$\begin{aligned} \nabla \cdot (\beta \nabla f) = & \frac{1}{h} \left[\beta_{i+1/2,j} \left(\frac{f_{i+1,j} - f_{i,j}}{h} \right) - \beta_{i-1/2,j} \left(\frac{f_{i,j} - f_{i-1,j}}{h} \right) \right] \\ & + \frac{1}{h} \left[\beta_{i,j+1/2} \left(\frac{f_{i,j+1} - f_{i,j}}{h} \right) - \beta_{i,j-1/2} \left(\frac{f_{i,j} - f_{i,j-1}}{h} \right) \right] \\ & - (F_R + F_L + F_B + F_T), \end{aligned} \quad (\text{E.19})$$

where F_R , F_L , F_B and F_T are additional terms that are non-zero when an interface is detected between the grid point (i, j) and its right, left, bottom or top neighbor, respectively. The coefficients $\beta_{i\pm 1/2,j}$ and $\beta_{i,j\pm 1/2}$ are equal to the local phase transport coefficient or fixed at $\hat{\beta}$ when the associated grid cell is crossed by the interface. For example, if an interface is located between grid points i and $i + 1$ as in the 1-D case and that the phase referred by Ω^+ is located on the right of the interface, F_R is given by

$$F_R = \frac{\hat{\beta} a_\Gamma}{h^2} + \frac{\hat{\beta} \left[\beta \frac{\partial f}{\partial x} \right]_\Gamma (1 - \theta)}{\beta^+ h} \quad (\text{E.20})$$

and $\beta_{i+\frac{1}{2}}$ is set to $\hat{\beta}$ as given by Eq. (E.14). The fraction θ of the grid cell on the left side of the interface can be estimated from the level set function as

$$\theta = \frac{|\phi_{i,j}|}{|\phi_{i+1,j}| + |\phi_{i,j}|}. \quad (\text{E.21})$$

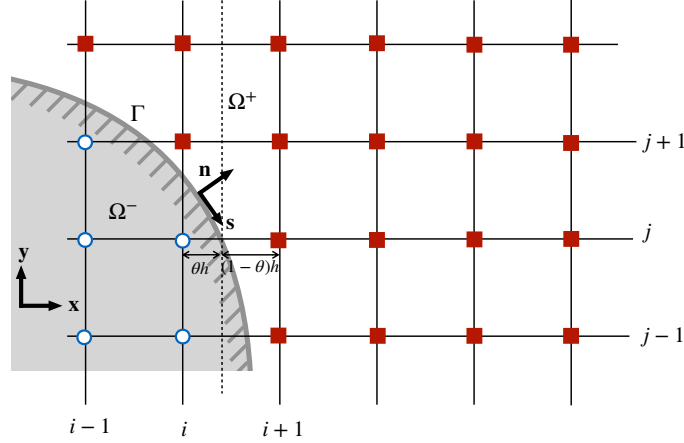


Figure E.2: Schematic plot of an interface immersed in two-dimensional cartesian grid (figure adapted from [49] with the courtesy of the first author).

Since the sharp interface method is applied individually along each cartesian direction, we need to express the jump conditions along x and y directions in terms of the normal and tangential derivatives:

$$\left[\beta \frac{\partial f}{\partial x} \right]_{\Gamma} = \left[\beta \frac{\partial f}{\partial n} \right]_{\Gamma} n_x + \left[\beta \frac{\partial f}{\partial s} \right]_{\Gamma} n_y \quad (\text{E.22})$$

$$\left[\beta \frac{\partial f}{\partial y} \right]_{\Gamma} = \left[\beta \frac{\partial f}{\partial n} \right]_{\Gamma} n_y - \left[\beta \frac{\partial f}{\partial s} \right]_{\Gamma} n_x. \quad (\text{E.23})$$

In Eqs. (E.22) and (E.23), the normal derivative jump is zero and, to ensure the continuity of the function f at the interface, we must have $\left[\frac{\partial f}{\partial s} \right]_{\Gamma} = 0$ so that

$\left[\beta \frac{\partial f}{\partial s} \right]_{\Gamma} = [\beta]_{\Gamma} \frac{\partial f}{\partial s} \Big|_{\Gamma}$. In [74], Liu et al. neglect the tangential derivative and simply project the normal jump along the two cartesian directions. In [111] and [119], the authors compute explicitly the term $\frac{\partial f}{\partial s} \Big|_{\Gamma}$ by interpolating the temperature or species concentration field on the surface of the particle. The tangential derivative is then obtained using centered finite differences with two neighbor points along the tangential direction. Here, we rather express the tangential derivative as

$$\frac{\partial f}{\partial s} \Big|_{\Gamma} = \frac{\partial f}{\partial x} \Big|_{\Gamma} n_y - \frac{\partial f}{\partial y} \Big|_{\Gamma} n_x. \quad (\text{E.24})$$

where the cartesian derivatives $\left. \frac{\partial f^+}{\partial x} \right|_{\Gamma}$ and $\left. \frac{\partial f^+}{\partial y} \right|_{\Gamma}$ are evaluated by interpolation on the fluid side of the interface as proposed in [49].

E.4 Validation: steady-state diffusion-reaction

We consider the two-dimensional steady-state reaction-diffusion equation for a given species of concentration C ²:

$$\nabla \cdot (\tilde{D} \nabla C) - \tilde{S} = 0, \quad (\text{E.25})$$

where the reaction source term $\tilde{S}$ is equal to $k_0 C$ in the solid (first-order catalytic reaction with rate constant k_0) and zero in the fluid. In the solid, Eq. (E.25) can be expressed in cylindrical coordinates and in a dimensionless form:

$$\hat{\nabla}_r^2 \hat{C}(\hat{r}) - Da_s \hat{C}(\hat{r}) = 0, \quad (\text{E.26})$$

where $Da_s = \frac{d_p^2 k_0}{D_s}$ is the solid-phase Damköhler number, $\hat{r} = \frac{r}{d_p}$, $\hat{\nabla}_r \cdot = d_p \nabla_r \cdot$ and $\hat{C} = \frac{C}{C_0}$, C_0 being the concentration at the surface of the particle. The analytical solution to Eq. (E.26) is given by

$$\hat{C}(\hat{r}) = \frac{J_0 \left(i \sqrt{Da_s} \hat{r} \right)}{J_0 \left(i \frac{\sqrt{Da_s}}{2} \right)}. \quad (\text{E.27})$$

where J_0 is the Bessel function of the first kind and order 0 and i is the unit imaginary number. In order to obtain $C = C_0$ at the surface of the particle, the ratio between the fluid and the solid diffusion coefficients is taken asymptotically large, e.g. $\frac{D_f}{D_s} = 10^4$, and the solid surface concentration C_0 is imposed as a Dirichlet boundary condition on the four sides of the domain. Figure E.3 compares the concentration profiles obtained with the SI method and a resolution $\frac{d_p}{h} = 40$ to the analytical solution given by Eq. (E.27). The agreement is very good, even for large values of Da_s where steep gradients appear in the solid phase.

For the case at $Da_s = 100$, we compare in Figure E.4 the performance of our sharp interface method to the diffuse interface method where the expression of the diffusion operator is not modified by the presence of the interface. It appears that the diffuse interface method captures with much less precision the location of the fluid/solid interface, especially at low resolution.

²The subscript α is omitted in this section for readability

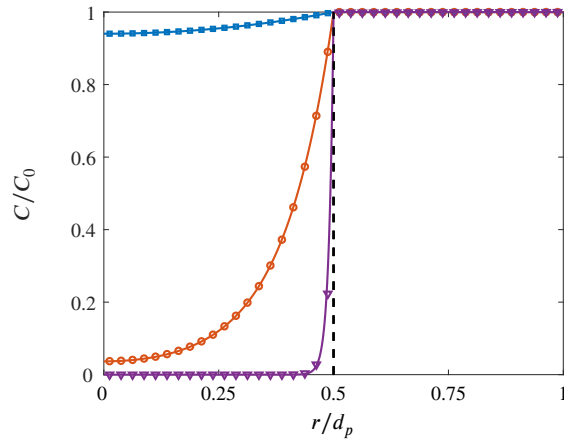


Figure E.3: Steady-state diffusion-reaction in a solid particle: radial concentration profile for $Da_s = 1$ ($\circ$), $Da_s = 100$ ($\square$) and $Da_s = 10\,000$ ($\triangle$). Solid lines correspond to the analytical solution Eq. (E.27) and symbols correspond to the results obtained using the sharp interface method with $\frac{d_p}{h} = 40$.

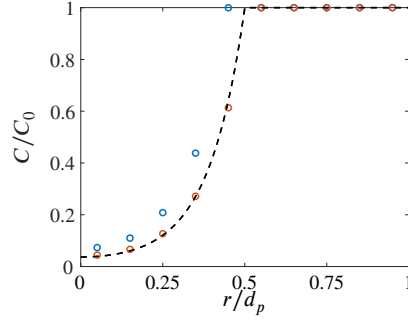
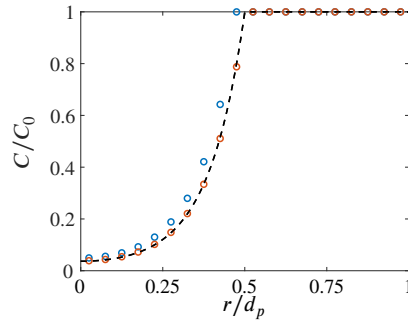
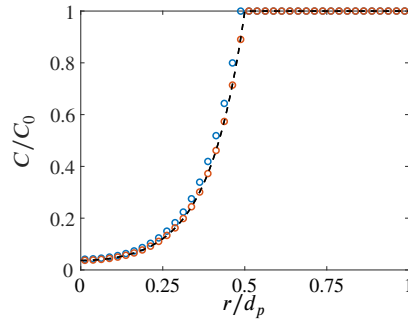
(a) $\frac{d_p}{h} = 10$ (b) $\frac{d_p}{h} = 20$ (c) $\frac{d_p}{h} = 40$

Figure E.4: Steady-state diffusion-reaction in a solid particle at $Da_s = 100$ and for increasing resolutions: comparison between the analytical solution (—) and the results obtained with the diffuse (●) and the sharp (○) interface methods.

Finally, the error made using each method with respect to the analytical solution can be computed and used to evaluate their convergence properties. In Figure E.5, we show the evolution of the L_2 and L_∞ errors associated to the two methods when the grid is refined. As expected, the error made using the DI method is larger than using the SI method and decreases less rapidly as the resolution increases. The convergence orders based on the L_2 and L_∞ errors are computed on each sub-interval (i.e. between 10 and 20 grid points per diameter, 20 and 30, etc.) for the two methods and are reported in Tables E.1 and E.2. The diffuse interface method is clearly first order while the sharp interface method is between first and second order.

Intervals	1	2	3	4	Average value
Diffuse interface	1.12	1.06	0.99	1.11	1.07
Sharp interface	1.61	1.90	1.88	1.72	1.78

Table E.1: Convergence orders evaluated from the L_2 error.

Intervals	1	2	3	4	Average value
Diffuse interface	0.84	0.92	0.96	0.97	0.92
Sharp interface	1.17	1.62	1.71	1.67	1.54

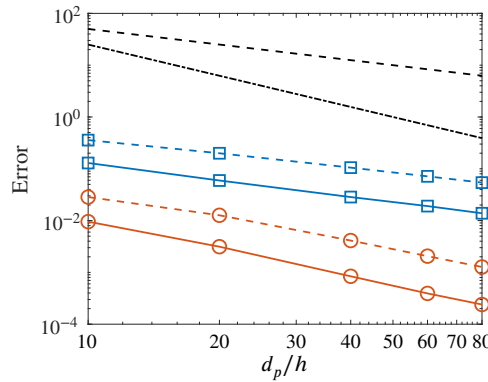
Table E.2: Convergence orders evaluated from the L_∞ error.

Figure E.5: Evolution of the L_2 (solid) and L_∞ (dashed) errors made with the diffuse (—■—) and the sharp (—○—) interface methods to solve the diffusion-reaction problem. First (---) and second (···) order convergence lines are also shown for comparison.

A penalization method for weakly compressible reacting gas-particle flows

We insert below the article "A penalization method for the simulation of weakly compressible reacting gas-particle flows with general boundary conditions", *Computers & Fluids*, 190 (2019), 294-307 [54], that we published in June 2019 about a Brinkman penalization method for gas-solid particle flows with variable density. This work was done before we switched to a direct-forcing immersed boundary method and it still rises some fundamental questions that we aim to address in the future. Note that this appendix has its own figure numbering and references that are unrelated to the global bibliography presented earlier.

A penalization method for the simulation of weakly compressible
reacting gas-particle flows with general boundary conditionsBaptiste Hardy^a, Juray De Wilde^a, Grégoire Winckelmans^b^aMaterials and Process Engineering, Institute of Mechanics, Materials and Civil Engineering, Université catholique de Louvain, Belgium^bThermodynamics and Fluid Mechanics, Institute of Mechanics, Materials and Civil Engineering, Université catholique de Louvain, Belgium

Abstract

In this paper, the Brinkman penalization method is extended to the weakly compressible formulation of the Navier-Stokes equations to study gas-particle flows with reactions and coupled heat and mass transfer. The weakly compressible approximation removes the acoustic modes from the solution while allowing a variable density. The Brinkman volume penalization method describes the solid phase as a porous medium with a vanishing permeability. The method is validated with literature benchmarks for a fixed or moving particle. Various reaction scenarios are then investigated. First, the capability of the method to deal with intra-particle diffusion and reaction is evaluated. The impact on the conversion of the particle Reynolds number based on the slip velocity is assessed, for a range of Reynolds numbers encountered in fluidization. Next, surface reactions are focused on, with infinite or finite rate. A Dirichlet-type condition is imposed on the particle surface to treat an infinite reaction rate and a high solid thermal conductivity while a finite-rate surface reaction requires Neumann and Robin surface conditions for the temperature and species mass fractions. The impact of density changes induced by heat release and molecular weight changes is assessed in these different cases. It is shown that the combination of the weakly compressible approximation and the penalization method allows to treat the presence of the solid phase and reactions in an efficient manner and to take into account the effects of compressibility in commonly encountered situations in reaction engineering.

Keywords: Penalization method, Direct Numerical Simulation, Gas-solid flows, Reacting flows, low-Mach approximation, Heat and mass transfer

1. Introduction

Gas-particle flows are encountered in a wide variety of natural phenomena and industrial applications. Among the latter, a special focus has been given to the modeling of fluidized bed reactors, due to their use in numerous processes: particle coating, base chemicals production, combustion, gasification,... Those are typically characterized by intense heat and mass transfer phenomena, in addition to complex flow structures caused by particle-particle and particle-fluid interactions. The simulation of large scale fluidized beds is typically performed by means of Two-Fluid Models (TFM), in which the solid phase is described in an Eulerian manner, or Discrete Element Methods (CFD-DEM), tracking each particle (or pseudo-particle) individually as a result of its interaction

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with the surrounding flow. In both approaches, closure laws are required to model the impact of the unresolved phenomena on the resolved scale of the flow. A number of correlations have been reported in the literature to obtain mass, momentum and heat transfer rates from known quantities, mostly based on experimental procedures. The weakness of these empirical correlations lies in their limited validity to mono-disperse particles, and their lack of local description [1]. Direct Numerical Simulation (DNS) of dense gas-particle flows has emerged as a powerful tool to derive closure relations based on fundamental physical grounds for the Two-Fluid and DEM-type models.

The detailed simulation of a flow with solid obstacles can be addressed in two ways: with a body conformal, or non-conformal grid. Methods based on body-fitting meshes, such as the arbitrary Lagrangian-Eulerian (ALE) finite-element method (FEM) [2], allow a straightforward treatment of the boundary conditions in the discretization process of the governing equations. Thanks to the alignment between the grid lines and the body boundaries, they also offer a better control of the grid resolution close to the body, where sharp gradients typically appear. However, the handling of more complex geometries or cases with a large fraction of the domain occupied by the dispersed phase makes the meshing process increasingly difficult. The treatment of moving bodies also requires a re-meshing at each time step and a projection of the solution onto the new grid. These two steps can drastically increase the complexity and the computational cost of the numerical method [3]. Immersed Boundary (IB) methods use non-conformal meshes. They have the advantage to use a fix grid, which reduces drastically the numerical complexity and cost of the meshing procedure. The counterpart is an increased effort to properly impose the boundary conditions on the surface of the body. The first continuous immersed boundary method was developed by Peskin [4] to simulate blood flows. IB methods are typically classified into continuous- and discrete-forcing methods. Continuous-forcing methods introduce an additional source term in the governing equations to impose the effect of the body on the fluid flow, typically using regularized delta functions. Uhlmann [5] extended Peskin's original formulation, allowing a more efficient treatment of rigid bodies. The main drawback of continuous formulations lies in the smearing of the body interface. Discrete-forcing (or sharp) IB methods, on the other hand, retain the accurate position of the interface and the forcing is introduced in the discretized form of the Navier-Stokes equations. Among those methods, the ghost-cell [6] and the cut-cell approaches [7, 8] are most widely used. The status of a ghost cell is determined from an extrapolation procedure (several schemes were derived by Majumdar [6]), and is later used in the Cartesian differentiation stencil to impose the desired boundary condition on the IB. The cut-cell (finite-volume) approach aims at guaranteeing strict local and global conservation of mass, heat and momentum by reshaping the fluid cells cut by the IB, discarding the part of the cell lying in the solid. The result of this operation is the creation of trapezoidal control volumes which leads to a finite-volume discretization of the Navier-Stokes equations. Some hybrid methods have also been developed, combining a diffuse IB method for the velocity field and a sharp interface method for the scalar fields in case of coupled mass or heat transfer between the solid and the fluid phase [9, 10].

The penalization method was first introduced by Arquies and Caltagirone [11] and belongs to the family of diffuse IB methods. In this approach, solid obstacles are modeled as porous media with vanishing permeability. Angot [12] provided a rigorous estimation of the convergence rate and error bounds for the penalization method. It was further extended to moving obstacles by Kolomenskiy et al. [13] and to scalar advection by Kadoch et al. [14]. A penalized vortex particle method was later proposed by Gazzola et al. [15] to handle deforming bodies with a non-divergence free velocity field. The penalization method has also been applied to compressible flows at both

low [16] and large [17] Mach number flows.

The new methodology proposed in this paper is to couple the penalization method with the low-Mach number (or weakly compressible) approximation [18]. The low-Mach number formulation of the Navier-Stokes equations removes the acoustic modes from the solution while still allowing a variable density. This approach appears particularly interesting for the treatment of reacting flows. Indeed, while strong temperature and species concentration gradients will appear and induce significant density fluctuations, the gas velocities are sufficiently low so that the condition $M^2 \ll 1$ is commonly satisfied. Abdelsamie et al. [19] studied two-phase turbulent reacting flows in the low-Mach approximation, using a direct-forcing IB method. Yet, the combination of the low Mach number approximation with the Brinkman penalization method appears particularly interesting for moderate Reynolds number flows. This paper presents the development of such a coupled approach as well as results obtained for general boundary conditions: Dirichlet-, Neumann- and Robin-type conditions corresponding to situations encountered in the field of reacting gas-solid flows. First, the governing equations are presented for the different types of boundary conditions. Then, the numerical method is developed and validated relatively to literature benchmarks. Finally, this new methodology is applied to the study of various situations encountered with reacting gas-solid flows, and the impact of compressibility effects is evaluated.

2. Governing equations

The computational domain Ω is split into a fluid part, Ω_f , and a solid part, Ω_s , formed by the ensemble of N_p particles

$$\Omega_s = \bigcup_{i=1}^{N_p} \Omega_{si}, \quad (1)$$

as sketched in Fig. 1.

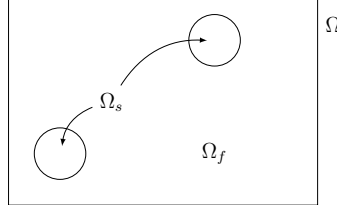


Figure 1: Sketch of the computational domain decomposition.

The fluid phase is considered as weakly compressible, i.e. acoustic modes are removed from the solution while the density is determined from the equation of state. The presence of the solid phase is treated via a Brinkman penalization method: the solid phase is tracked using a mask function, and additional source terms are added to the fluid phase governing equations to enforce the interface boundary conditions.

We first recall the low Mach number equations for the fluid phase. The penalization method is then extended to the framework of weakly compressible flows, and for both Dirichlet and Neumann- or Robin-type boundary conditions.

2.1. The low-Mach number approximation

When the compressible Navier-Stokes equations are taken to the limit of vanishing Mach number, the weakly compressible Navier-Stokes equations are obtained (a rigorous derivation can be found in [18, 20]):

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \quad (2)$$

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla \tilde{p} + \nabla \cdot \boldsymbol{\tau} \quad (3)$$

$$\rho c_p \left(\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T \right) = \nabla \cdot (\kappa \nabla T) + \sum_{k=1}^{N_s} h_k \dot{w}_k + \frac{dp_0}{dt} \quad (4)$$

$$\rho \left(\frac{\partial Y_k}{\partial t} + \mathbf{u} \cdot \nabla Y_k \right) = -\nabla \cdot (\rho Y_k \mathbf{v}_k) - \dot{w}_k, \quad (5)$$

with the shear stress tensor, $\boldsymbol{\tau}$, defined as

$$\boldsymbol{\tau} = \mu \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T - \frac{2}{3} (\nabla \cdot \mathbf{u}) \mathbf{I} \right). \quad (6)$$

In Eqs. (2)-(6), ρ is the fluid density, $\mathbf{u}$ the velocity field, T the temperature, Y_k the mass fraction of species k ($k = 1, \dots, N_s$), $\mathbf{I}$ the identity tensor, $\tilde{p}$ the dynamic pressure, p_0 the space-uniform background pressure, μ the dynamic viscosity, c_p the fluid specific heat, κ the fluid heat conductivity, h_k the enthalpy of formation of species k , $\dot{w}_k$ its volumetric consumption rate and $\mathbf{v}_k$ its diffusion velocity. Assuming that all species have equal diffusivity $\mathcal{D}$, the diffusion velocity of species k is modeled as

$$\mathbf{v}_k = -\frac{\mathcal{D}}{Y_k \bar{W}} \nabla (Y_k \bar{W}), \quad (7)$$

with $\bar{W}$ the average molecular weight of the mixture:

$$\bar{W} = \left(\sum_{k=1}^{N_s} \frac{Y_k}{W_k} \right)^{-1}. \quad (8)$$

In Eqs. (2)-(5), the heat generated by viscous dissipation and the heat flux induced by species diffusion have been neglected.

A dimensional analysis of the compressible momentum equation shows that the spatial gradient of the pressure p is $\mathcal{O}(M^2)$ [18, 21] so that it can be decomposed as

$$p(\mathbf{x}, t) = p_0(t) + \underbrace{\tilde{p}(\mathbf{x}, t)}_{\mathcal{O}(M^2)} \quad (9)$$

where $p_0(t)$ is spatially uniform and $\tilde{p}(\mathbf{x}, t)$ is the fluctuating part of the pressure which drives the fluid dynamics. It follows from the low-Mach number approximation that the thermodynamic pressure can be linked to the temperature through the equation of state

$$p_0 = \rho T \frac{\mathcal{R}}{\bar{W}} \quad (10)$$

with $\mathcal{R}$ the universal gas constant.

When the domain has an open boundary (e.g. inflow/outflow problems), p_0 is fixed by the atmospheric conditions. In the case of a closed domain (e.g. combustion in a closed enclosure), the total mass $M_0 = \int_V \rho dV$ remains constant in time. Integrating both sides of Eq. (10) leads to

$$p_0 = \frac{M_0 \mathcal{R}}{\int_V \left(\frac{\bar{W}}{T} \right) dV}. \quad (11)$$

2.2. The penalization method

The volume penalization method was firstly and mostly employed to simulate incompressible flows with obstacles. It was further extended to compressible flows by Liu and Vasilyev [16]. The simple conservation of the continuity equation inside a penalized obstacle was found to cause unacceptable errors, leading these authors to propose an additional penalization on the continuity equation. Their method was limited to Dirichlet boundary conditions on the flow variables at the surface of obstacles, and it was subsequently extended by Brown-Dymkoski et al. [22] to Neumann- and Robin-type boundary conditions. In the following, the penalization method is developed in the framework of the low-Mach number approximation, and for both Dirichlet and Neumann-Robin type surface conditions.

The solid phase is tracked through a mask function, χ :

$$\chi(\mathbf{x}, t) = \begin{cases} 1 & \text{if } \mathbf{x} \in \Omega_s, \\ 0 & \text{elsewhere.} \end{cases} \quad (12)$$

2.2.1. Dirichlet boundary condition

The penalized low-Mach number equations with prescribed velocity $\mathbf{u}_s$, temperature T_s and composition $Y_{k,s}$ on the particle surface, are

$$\frac{\partial \rho}{\partial t} = - \left[1 + \chi \left(\frac{1}{\Phi} - 1 \right) \right] \nabla \cdot (\rho \mathbf{u}) \quad (13)$$

$$\frac{\partial}{\partial t} (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = - \nabla \tilde{p} + \nabla \cdot \boldsymbol{\tau} - \chi \left(\rho \frac{(\mathbf{u} - \mathbf{u}_s)}{\Delta \tau} \right) \quad (14)$$

$$\rho c_p \left(\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T \right) = \nabla \cdot (\kappa \nabla T) + \sum_{k=1}^{N_s} h_k \dot{w}_k + \frac{dp_0}{dt} - \chi \left(\rho c_p \frac{(T - T_s)}{\Delta \tau} \right) \quad (15)$$

$$\rho \left(\frac{\partial Y_k}{\partial t} + \mathbf{u} \cdot \nabla Y_k \right) = - \nabla \cdot (\rho Y_k \mathbf{v}_k) - \dot{w}_k - \chi \left(\rho \frac{(Y_k - Y_{k,s})}{\Delta \tau} \right) \quad (16)$$

with Φ a very small dimensionless number and $\Delta \tau$, a small number with dimensions of a time.

2.2.2. Neumann and Robin boundary condition

In [22], Brown-Dymkoski et al. introduced the so-called characteristic based volume penalization (CBVP) method for general boundary conditions by introducing hyperbolic penalization terms with inward pointing characteristics. This opened the way to more general boundary conditions on solid interfaces. In the present work, the CBVP method is extended to low Mach number Navier-Stokes equations and further used to study realistic cases such as surface reactions with

heat release. In [22], the authors remove from the solution the right-hand-side containing the physical terms inside the penalized obstacle when a Dirichlet boundary condition is prescribed for one of the flow variables (e.g. no-slip condition on the velocity). We here choose to stick to the original formulation [12] and preserve the constitutive equations inside the obstacle, which ensures the smoothness of the solution, such that Eqs. (13) and (14) are unchanged. Let us now consider the general case of a Robin-type boundary condition imposed on the scalar flow variable ϕ at the particle surface:

$$\alpha\phi + \beta\frac{\partial\phi}{\partial n} = q(\mathbf{x}, t) \quad (17)$$

with α a physical quantity with units inverse of a length and β a dimensionless quantity. The general conservation equation $\frac{\partial\phi}{\partial t} = \text{RHS}$, where RHS is the right-hand side of the conservation equation which governs the time variation of ϕ in the fluid phase, is penalized as

$$\frac{\partial\phi}{\partial t} = (1 - \chi)\text{RHS} - \frac{\chi}{\eta_c} (\alpha\phi + \beta(\hat{\mathbf{n}} \cdot \nabla\phi) - q), \quad (18)$$

with η_c , the penalization parameter such that $1/\eta_c$ has units of a velocity. The unit normal vector to the surface, $\hat{\mathbf{n}}$, is pointing inward the obstacle to propagate information from the surface. It is defined everywhere inside the obstacle as

$$\hat{\mathbf{n}} = \frac{\nabla d}{|\nabla d|}, \quad (19)$$

where d is the distance to the surface function.

A Neumann-type boundary condition is treated identically, with $\alpha = 0$.

The penalized weakly compressible equations for general Robin-type boundary conditions on temperature and species mass fractions are then taken as

$$\frac{\partial T}{\partial t} = (1 - \chi) \left(-\mathbf{u} \cdot \nabla T + \frac{1}{\rho c_p} \nabla \cdot (\kappa \nabla T) + \frac{dp_0}{dt} + \sum_{k=1}^{N_s} h_k \dot{w}_k \right) - \frac{\chi}{\eta_c} (\alpha_T T + \beta_T (\hat{\mathbf{n}} \cdot \nabla T) - q) \quad (20)$$

$$\frac{\partial Y_k}{\partial t} = (1 - \chi) \left(-\mathbf{u} \cdot \nabla Y_k - \frac{1}{\rho} \nabla \cdot (\rho Y_k \mathbf{v}_k) - \dot{w}_k \right) - \frac{\chi}{\eta_c} (\alpha_{Y_k} Y_k + \beta_{Y_k} (\hat{\mathbf{n}} \cdot \nabla Y_k) - q_k). \quad (21)$$

An issue arises when closed obstacles such as cylinders or spheres are considered. Indeed, characteristics propagate information from the surface inwards, and they will meet at any interior point equidistant from two points of the surface, carrying conflicting information. This problem can be solved as described in [22] and sketched in Fig. 2: the additional hyperbolic penalization term is only added in a small region close to the surface, yet large enough to support the differentiation stencil imposing the desired condition on the particle boundary. The core region is simply governed by artificial diffusion. The use of upwind differentiation schemes in the hyperbolic region avoids the crossing of the hyperbolic-diffusive discontinuity which would result in a strong degradation of the physical solution.

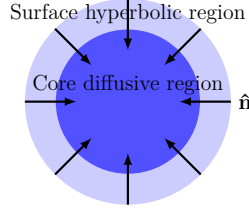


Figure 2: Sketch of the hyperbolic surface region and diffusive core region in CBVP, with inward pointing unit normal vector.

2.2.3. Coupled solid-fluid heat and mass transfer

When the interior of the solid phase undergoes a catalytic diffusion-reaction process (i.e. the reaction occurs in the solid phase only), a pseudo-continuum description of the solid phase can be adopted, and the penalization mask can be used to modify the value of the transport coefficients and source terms according to the current phase, such that Eqs. (4) and (5) are modified as

$$\frac{\partial T}{\partial t} = -\mathbf{u} \cdot \nabla T + \frac{1}{\tilde{\rho}\tilde{c}_p} \nabla \cdot (\tilde{\kappa} \nabla T) + \chi \sum_{k=1}^{N_s} h_k \dot{w}_k + (1 - \chi) \frac{dp_0}{dt} \quad (22)$$

$$\frac{\partial Y_k}{\partial t} = -\mathbf{u} \cdot \nabla Y_k + \frac{1}{\tilde{\rho}} \nabla \cdot \left(\frac{\tilde{\rho} \tilde{D}}{\tilde{W}} \nabla (Y_k \tilde{W}) \right) - \chi \dot{w}_k \quad (23)$$

where each physical quantity " $\tilde{\cdot}$ " has the value of the corresponding phase:

$$\tilde{f} = \chi f_s + (1 - \chi) f \quad (24)$$

with f , the value of the quantity in the fluid phase and f_s its value in the solid phase.

2.3. Solid-phase equations

When allowed to move, each particle is tracked in a Lagrangian way by solving the Newton-Euler equations of motion:

$$m_s \dot{\mathbf{U}}_s = \mathbf{F}_{f \rightarrow s} \quad (25)$$

$$I_s \dot{\boldsymbol{\omega}}_s = \mathbf{T}_{f \rightarrow s}, \quad (26)$$

with m_s , the mass of the particle, I_s its moment of inertia, $\mathbf{U}_s$ its translational velocity and $\boldsymbol{\omega}_s$ its angular velocity. The velocity of the particle at a distance $\mathbf{r}$ from its center is then obtained as the combination of the translational and rotational contributions:

$$\mathbf{u}_s = \mathbf{U}_s + \boldsymbol{\omega}_s \times \mathbf{r}. \quad (27)$$

The interfacial force, $\mathbf{F}_{f \rightarrow s}$, and torque, $\mathbf{T}_{f \rightarrow s}$, are obtained through integration of the penalization term over the volume of the body:

$$\begin{aligned}
 \mathbf{F}_{f \rightarrow s} &= - \oint_{\partial\Omega_s} \boldsymbol{\sigma} \cdot \hat{\mathbf{n}} dS \\
 &= \int_{\Omega_s} \nabla \cdot \boldsymbol{\sigma} dV \\
 &= \int_{\Omega_s} \rho \frac{d\mathbf{u}}{dt} dV + \int_{\Omega_s} \chi \rho \frac{(\mathbf{u} - \mathbf{u}_s)}{\Delta\tau} dV \\
 &= \dot{\mathbf{U}}_s \int_{\Omega_s} \rho dV + \int_{\Omega_s} \chi \rho \frac{(\mathbf{u} - \mathbf{u}_s)}{\Delta\tau} dV.
 \end{aligned} \tag{28}$$

As detailed in [5] for the incompressible case, the rigid body assumption allows us to extract the particle acceleration, $\dot{\mathbf{U}}_s$, from the first integral term, the extension to the present compressible situation is straightforward.

The interfacial torque is obtained in a similar way:

$$\begin{aligned}
 \mathbf{T}_{f \rightarrow s} &= - \int_{\partial\Omega_s} \mathbf{r} \times (\boldsymbol{\sigma} \cdot \hat{\mathbf{n}}) dS \\
 &= \int_{\Omega_s} (\mathbf{r} \wedge \nabla \cdot \boldsymbol{\sigma}) dV \\
 &= \frac{d}{dt} \int_{\Omega_s} (\mathbf{r} \wedge \rho \mathbf{u}) dV + \int_{\Omega_s} \left(\mathbf{r} \wedge \chi \rho \frac{(\mathbf{u} - \mathbf{u}_s)}{\Delta\tau} \right) dV \\
 &= \dot{\boldsymbol{\omega}}_s \int_{\Omega_s} \rho r^2 dV + \int_{\Omega_s} \left(\mathbf{r} \wedge \chi \rho \frac{(\mathbf{u} - \mathbf{u}_s)}{\Delta\tau} \right) dV.
 \end{aligned} \tag{29}$$

3. Numerical method

We use a predictor-corrector scheme to integrate the continuity equations, similar to those developed in [23, 24, 25]. As summarized in the review paper of Knikker [26], different approaches can be adopted in the sequence chosen for solving the conservation equations. In [23], Najm et al. solve the conservation equations for the density and the mass fractions before updating the temperature from the equation of state. In [24], Lessani et al. split the thermo-chemical system by solving the species continuity equations once the flow field has been advanced, assuming constant molecular weight. In this paper, the temperature and species mass fractions are first integrated. The density is subsequently obtained from state law and the velocity field can finally be updated. Second-order schemes are used for the evaluation of spatial derivatives. A classical staggered mesh is employed: the scalar quantities and the diagonal shear stresses are stored at the center of the cell, the velocities, heat and mass fluxes on the faces of the cell, and the off-diagonal shear stresses on the cell vertices.

In the following, $\mathcal{P}_\phi$ denotes the penalization source term on the quantity ϕ (temperature or species mass fraction), no matter whether it corresponds to a Dirichlet or to a Neumann/Robin-type boundary condition.

3.1. Predictor

The predictor step uses an Adams-Bashforth scheme of order 2 (AB2) for the time integration of the convective terms, and an Euler scheme for the diffusive and source terms, as well as for the

penalization term.

1. Integrate the energy and species transport equations

One first computes a predictor for the temperature

$$\frac{(T^* - T^n)}{\Delta t} = \left(\frac{3}{2} C_T^n - \frac{1}{2} C_T^{n-1} \right) + \frac{1}{\rho^n c_p} \left(D_T^n + S_T^n + \frac{dp_0^n}{dt} + \mathcal{P}_T \right) \quad (30)$$

where

- $C_T = -\mathbf{u} \cdot \nabla T$
- $D_T = \nabla \cdot (\kappa \nabla T)$
- $S_T = \sum_{k=1}^{N_s} h_k \dot{w}_k$
- $\frac{dp_0^n}{dt} = \frac{p_0^n - p_0^{n-1}}{\Delta t}$.

Similarly for the species transport equation:

$$\frac{(Y_k^* - Y_k^n)}{\Delta t} = \left(\frac{3}{2} C_{Y_k}^n - \frac{1}{2} C_{Y_k}^{n-1} \right) + \frac{1}{\rho^n} (D_{Y_k}^n + S_{Y_k}^n + \mathcal{P}_{Y_k}) \quad (31)$$

where

- $C_{Y_k} = -\mathbf{u} \cdot \nabla Y_k$
- $D_{Y_k} = -\nabla \cdot (\rho Y_k \mathbf{v}_k)$
- $S_{Y_k} = -\dot{w}_k$.

Then, the mean molecular weight can be updated based on Eq. (8)

2. Update the thermodynamic pressure

For an open domain, $p_0^* = p_{atm}$. For a closed domain, p_0^* is deduced from Eq. (11).

3. Update the density.

Use Eq. (10) to obtain ρ^* from T^* and $\bar{W}^*$

4. Integrate the momentum equation using a two-step projection method

The integration of the momentum equation is based on Chorin's two-step projection method [27]. An intermediate velocity field $\hat{\mathbf{u}}$ is first computed

$$\frac{(\rho^* \hat{\mathbf{u}} - \rho^n \mathbf{u}^n)}{\Delta t} = \underbrace{\left(\frac{3}{2} \mathbf{C}_{\mathbf{u}}^n - \frac{1}{2} \mathbf{C}_{\mathbf{u}}^{n-1} \right) + \nabla \cdot \boldsymbol{\tau}^n - \nabla \tilde{p}^n}_{\triangleq \text{RHS}} - \chi \left(\frac{\rho^* (\hat{\mathbf{u}} - \mathbf{u}_s)}{\Delta \tau} \right), \quad (32)$$

where $\mathbf{C}_{\mathbf{u}} = -\nabla \cdot (\rho \mathbf{u} \mathbf{u})$.

In the case of a Dirichlet boundary condition, the penalization term can be treated implicitly in a straightforward way, which allows the use of a very large ratio $\frac{\Delta t}{\Delta \tau} \gg 1$, ensuring an accurate enforcement of the boundary condition without constraining the time step to a

small value. In the present work, we used a ratio $\frac{\Delta t}{\Delta \tau} = 1.0 \cdot 10^4$. The intermediate velocity field is then obtained as

$$\hat{\mathbf{u}} = \left(\left(\frac{\rho^n}{\rho^*} \right) \mathbf{u}^n + \frac{1}{\rho^*} \Delta t \text{ RHS} + \left(\frac{\Delta t}{\Delta \tau} \right) \mathbf{u}_s \right) / \left(1 + \chi \left(\frac{\Delta t}{\Delta \tau} \right) \right). \quad (33)$$

The implicit integration of the penalization term is similarly performed for scalar quantities in Eqs. (30) and (31) when a Dirichlet condition is imposed on the solid surface ($\mathcal{P}_\phi = \mathcal{P}_\phi^*$), while it is treated explicitly for Neumann- and Robin-type boundary conditions ($\mathcal{P}_\phi = \mathcal{P}_\phi^n$). The intermediate velocity field $\hat{\mathbf{u}}$ does not satisfy the continuity equation and needs to be further corrected:

$$\frac{(\rho^* \mathbf{u}^* - \rho^* \hat{\mathbf{u}})}{\Delta t} = -\nabla p', \quad (34)$$

with $p' = \bar{p}^* - \bar{p}^n$ the pressure correction field, obtained as the solution of a Poisson equation.

From there, the constraint coming from the continuity equation can be imposed in two ways [28]:

- (a) A first approach consists in using the conservative form of the continuity equation by taking the divergence of the *momentum* ($\rho \mathbf{u}$) in order to satisfy the mass conservation constraint. This leads to a Poisson equation, requiring the evaluation of $\left(\frac{\partial \rho}{\partial t} \right)$. However, it has been reported in the literature [29, 28, 20] that the time derivative of the density is a source of instability, limiting the method to moderate density ratios.
- (b) A second approach uses the continuity equation in its non-conservative form to impose the divergence of the *velocity* $\mathbf{u}$. This method turns out to be more robust and shows good stability properties when dealing with strong thermal and density gradients. The main drawback is that one needs to solve a numerically challenging variable-coefficient Poisson equation.

The first method has been used in the current work. The divergence operator is applied to both sides of Eq. (34):

$$\frac{1}{\Delta t} (\nabla \cdot (\rho^* \mathbf{u}^*) - \nabla \cdot (\rho^* \hat{\mathbf{u}})) = -\nabla^2 p'. \quad (35)$$

The first term on the left-hand side is obtained from the continuity Eq. (13),

$$\nabla \cdot (\rho^* \mathbf{u}^*) = \frac{-\left(\frac{\partial \rho}{\partial t} \right)^*}{\left[1 + \chi \left(\frac{1}{\Phi} - 1 \right) \right]} \stackrel{\text{3BDF}}{=} -\frac{(3\rho^* - 4\rho^n + \rho^{n-1})}{2\Delta t} / \left[1 + \chi \left(\frac{1}{\Phi} - 1 \right) \right], \quad (36)$$

where the time derivative of density is evaluated with a 3 points backward difference scheme (3BDF), while the second term is evaluated using the divergence of $(\rho^* \hat{\mathbf{u}})$ obtained from (32). The parameter Φ is fixed to $1.0 \cdot 10^{-4}$ for all subsequent simulations. The resulting Poisson equation is solved using a conjugate gradient solver preconditioned with a multi-grid method.

3.2. Corrector

If the integration is stopped after the predictor step, the method will show very poor time convergence since the predicted value for the density, ρ , is never corrected. A corrector step is hence added.

1. Integrate the energy and species transport equations

For the correction step, we use a second-order "quasi Crank-Nicolson" scheme to advance the scalar quantities of the energy and species transport equations:

$$\begin{aligned} \frac{(T^{n+1} - T^n)}{\Delta t} &= \frac{1}{2} \left(C_T^n + \frac{1}{\rho^n c_p} (D_T^n + S_T^n) \right) + \frac{1}{2} \left(C_T^* + \frac{1}{\rho^* c_p} (D_T^* + S_T^*) \right) \\ &\quad + \frac{1}{\rho^* c_p} \left(\frac{p_0^n - p_0^{n-1}}{\Delta t} \right) + \mathcal{P}_T \end{aligned} \quad (37)$$

$$\frac{(Y_k^{n+1} - Y_k^n)}{\Delta t} = \frac{1}{2} \left(C_{Y_k}^n + \frac{1}{\rho^{n+1}} (D_{Y_k}^n + S_{Y_k}^n) \right) + \frac{1}{2} \left(C_{Y_k}^* + \frac{1}{\rho^{n+1}} (D_{Y_k}^* + S_{Y_k}^*) \right) + \mathcal{P}_{Y_k}, \quad (38)$$

an the mean molecular weight is subsequently updated using Eq. (8).

2. Update the thermodynamic pressure

For an open domain, $p_0^{n+1} = p_{atm}$. For a closed domain, p_0^{n+1} is deduced from Eq. (11).

3. Update the density.

Use Eq. (10) to obtain ρ^{n+1} from T^{n+1} and $\bar{W}^{n+1}$.

4. Integrate the momentum equation using a two-step projection method.

Similarly to what was done in the predictor step, we first compute the intermediate velocity field, $\tilde{\mathbf{u}}$:

$$\frac{(\rho^{n+1} \tilde{\mathbf{u}} - \rho^n \mathbf{u}^n)}{\Delta t} = \left(\frac{3}{2} \mathbf{C}_{\mathbf{u}}^n - \frac{1}{2} \mathbf{C}_{\mathbf{u}}^{n-1} \right) + \nabla \cdot \boldsymbol{\tau}^n - \nabla \tilde{p}^n - \chi \left(\frac{\rho^{n+1} (\tilde{\mathbf{u}} - \mathbf{u}_s)}{\Delta \tau} \right) \quad (39)$$

before enforcing the mass conservation

$$\frac{(\rho^{n+1} \mathbf{u}^{n+1} - \rho^{n+1} \tilde{\mathbf{u}})}{\Delta t} = -\nabla p', \quad (40)$$

with $p' = \tilde{p}^{n+1} - \tilde{p}^n$, obtained as the solution of the Poisson equation

$$\frac{1}{\Delta t} \left(\nabla \cdot (\rho^{n+1} \mathbf{u}^{n+1}) - \nabla \cdot (\rho^{n+1} \tilde{\mathbf{u}}) \right) = -\nabla^2 p', \quad (41)$$

where

$$\nabla \cdot (\rho^{n+1} \mathbf{u}^{n+1}) = \frac{-\left(\frac{\partial \rho}{\partial t}\right)^{n+1}}{\left[1 + \chi \left(\frac{1}{\Phi} - 1\right)\right]} = -\frac{(3\rho^{n+1} - 4\rho^n + \rho^{n-1})}{2\Delta t} \Big/ \left[1 + \chi \left(\frac{1}{\Phi} - 1\right)\right]. \quad (42)$$

4. Non-reactive case studies

In order to first validate the flow part of the present methodology, some benchmark cases used for incompressible and compressible flows are reproduced using our weakly compressible code. The fluid-phase Prandtl number is $Pr = \frac{\mu_0 c_{p0}}{\kappa_0} = 0.7$, with μ_0 , c_{p0} and κ_0 , respectively the dynamic viscosity, specific heat and conductivity of the fluid at the reference inlet temperature T_0 .

4.1. Flow past a fixed cylinder

A circular disk with diameter d_p is placed in a channel with dimensions $30d_p \times 30d_p$ and slip walls, at a distance $10d_p$ from the inflow, where a uniform velocity profile u_∞ is imposed. The flow past the disk is computed for three different particle Reynolds number: $Re_p = \frac{\rho_0 u_\infty d_p}{\mu_0} = 40$, $Re_p = 100$ and $Re_p = 1000$, ρ_0 being the reference fluid density at T_0 . Unless otherwise specified, the resolution used for all the subsequent simulations is $d_p = 30h$, with h the grid size.

4.1.1. $Re_p = 40$, $T_s = T_0$

At $Re_p = 40$, the flow is steady. If the particle temperature T_s is set equal to the reference temperature T_0 and that adiabatic conditions are imposed on the channel walls, the temperature and hence the density are uniform and constant throughout the simulation. The drag coefficient as well as different geometrical features of the flow (illustrated in Fig. 3) are extracted and compared to the literature in Table 1. Both experimental results ([30, 31]) and numerical studies have been reported. The results from the present study agree reasonably well with the reference results. The slightly high value reported for our drag coefficient with respect to other studies must be attributed to confinement effects.

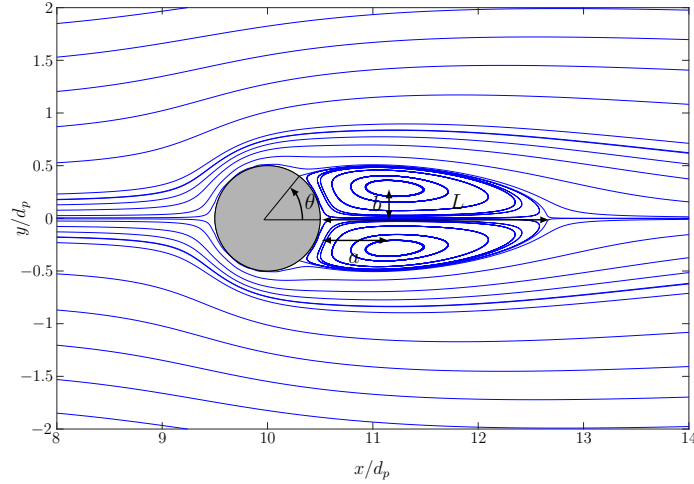


Figure 3: Streamlines of the flow past a cylinder at $Re_p = 40$ and definition of geometrical characteristics of the flow.

Study	C_D	$\frac{a}{d_p}$	$\frac{b}{d_p}$	$\frac{L}{d_p}$	θ
Present	1.57	0.73	0.57	2.15	53.1°
Bigay et al. [32]	1.57	0.70	0.59	2.22	50.3°
Canuto & Taira [33]	1.54	0.72	0.59	2.24	53.8°
Linnick & Fasel [34]	1.52	0.72	0.60	2.28	53.6°
Denis & Chang [35]	1.52	—	—	2.35	53.8°
Tritton* [30]	1.59	—	—	—	—
Bouard & Countanceau* [31]	—	0.76	0.59	2.13	53.8°

Table 1: Flow past a fixed cylinder at $Re_p = 40$: drag coefficient and geometrical flow features. Superscript ** indicates experimental studies.

4.1.2. $Re_p = 40$, $T_s \neq T_0$

We here investigate the impact of the particle surface temperature on the drag coefficient and Nusselt number. Values of drag and heat transfer coefficients in forced convection past a cylinder are provided in the literature or correlated for a range of low to moderate Reynolds numbers, under the incompressible approximation. On the other hand, the effect of compressibility with non-zero Mach number flows has also been studied [36, 33] and values of drag coefficients are reported for a range of Reynolds and Mach numbers. The effect of density fluctuations resulting from temperature and composition changes on momentum, heat and mass transfer has, however, not been studied separately so far.

A set of numerical experiments has been performed with increasing values of the ratio T_s/T_0 . Fig. 4 shows the extracted particle drag coefficient and Nusselt number. The Nusselt number point at $T_s/T_0 = 1$ actually corresponds to that extracted from an incompressible simulation with $T_s \neq T_0$ (since no heat transfer occurs for a unit ratio). Yet, it can be considered as the limit Nusselt number of the present weakly compressible case for a vanishing driving force. The value of the Nusselt number extracted from this incompressible simulation is $Nu = 3.257$, i.e. a difference of 2.63 % with respect to the value obtained using the Churchill-Bernstein correlation [37]:

$$\overline{Nu} = 0.3 + \frac{0.62Re_p^{1/2}Pr^{1/3}}{[1 + (0.4/Pr)^{2/3}]^{1/4}} \left[1 + \left(\frac{Re_p}{282000} \right)^{5.8} \right]^{4/5} = 3.345. \quad (43)$$

Fig. 4 further shows that a larger ratio T_s/T_0 results in an increase of the drag and a decrease of the heat transfer coefficient, and in a quite linear way.

4.1.3. $Re_p = 100$, $T_s = T_0$

At $Re_p = 100$, the problem is unsteady with the onset of the Von-Karman vortex shedding. Once the flow has reached a statistically stationary state, the time-averaged drag coefficient $\overline{C_D}$ and the Strouhal number, $St = \frac{f_L d_p}{u_\infty}$, based on the oscillation frequency of the lift coefficient, f_L , are reported in TABLE 2, together with reference results. Again, good agreement is found, demonstrating the ability of our method to capture accurately moderate Reynolds number unsteady flows.

4.1.4. Heated cylinder at $Re_p = 1000$

The implementation of the CBVP method to impose Neumann- and Robin-type boundary conditions is here validated by simulating the flow past a heated cylinder at $Re_p = 1000$. A

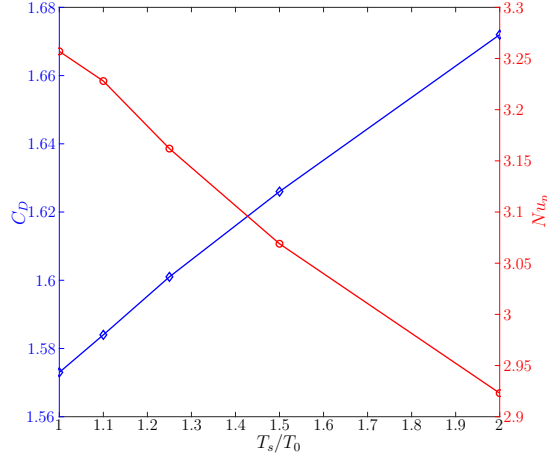


Figure 4: Evolution of the drag coefficient ($-\diamond$) and Nusselt number ($-\circ$) with the solid particle temperature.

Study	$\overline{C_D}$	St
Present	1.34	0.170
Canuto & Taira [33]	1.34	0.167
Mittal et al. [38]	1.35	0.165
Apte et al. [39]	1.36	0.165

Table 2: Flow past a fixed cylinder at $Re_p = 100$: time-averaged drag coefficient and Strouhal number.

flux $\frac{\partial T}{\partial n} = 1.5 (T_0/d_p)$ is imposed on the particle surface using Eq. (20). In their paper, Brown-Dymkoski et al. [22] use a Mach number $M = 0.20$ as they consider the fully compressible Navier-Stokes equations. Yet, the usual condition $M^2 \ll 1$ is still legitimate, such that the present low-Mach approximation should reproduce fairly correctly the results obtained in [22]. The domain considered has a size $[0, 12]d_p \times [-3, 3]d_p$ and the particle is positioned at $(3, 0)d_p$. The penalization parameter η_c is fixed so that $\eta_c u_\infty = 0.05$. Fig. 6a shows a close-up view of the resulting instantaneous temperature field. A vertical cut in the temperature field is extracted and plotted in Fig. 6b to verify the proper enforcement of the desired boundary condition $q = 1.5 T_0/d_p$. The time evolution of the drag and lift coefficients are given in Fig. 7. The average drag coefficient is $\overline{C_D} = 1.74$ and the Strouhal number based on the oscillation frequency of the drag coefficient is $St = 0.257$, compared to $St = 0.245$ obtained by Brown-Dymkoski et al. [22]. Our slightly higher St could be due to our stronger confinement effects and/or our lower value of $\eta_c u_\infty$.

4.2. Sedimentation of a single particle

In order to validate the fluid-solid coupling of the present method, the classical test case of a cylinder sedimenting in a viscous fluid is reproduced. A no-slip condition is imposed on the walls of the channel. The cylinder accelerates under the single action of gravity until it reaches its terminal

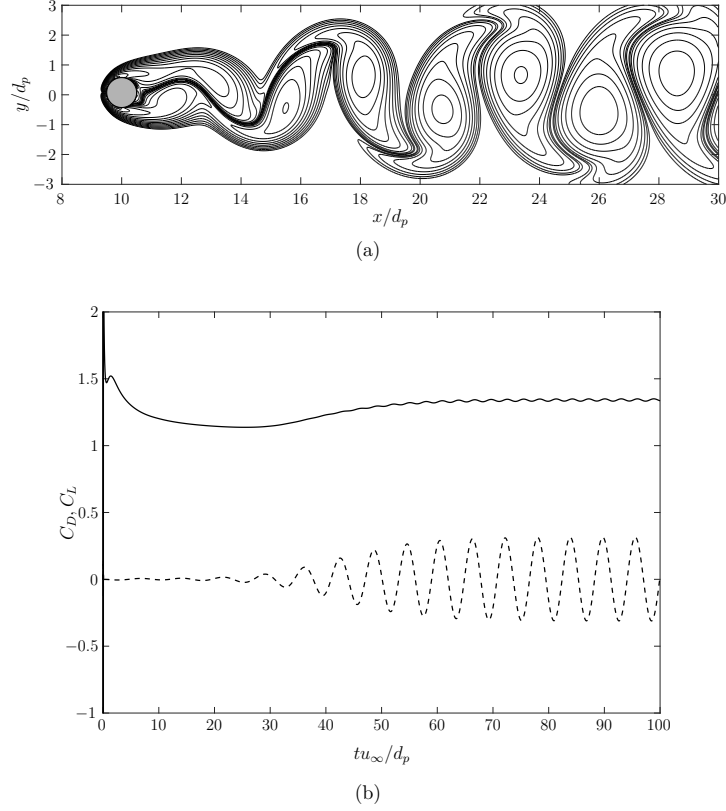


Figure 5: Flow past a cylinder at $Re_p = 100$. (a) Iso-contours of the dimensionless vorticity $\frac{|\omega|d_p}{u_\infty} = 10^a$, with $a = -2.0, -1.75, -1.50, \dots, 2.0$. (b) Time evolution of drag (solid line) and lift (dashed line) coefficients.

velocity, v_t . The collision of the particle with the bottom wall is part of the simulation and the collision model employed is based on repulsion forces as described by Feng and Michaelides in [40]. The geometrical and physical parameters are identical to those employed by Glowinski et al. [41] who define the reference length l_0 as the half-width of the channel, the reference velocity u_0 as $\sqrt{\frac{gl_0}{981}}$, with g the gravitational acceleration, so that the reference time is $t_0 = \frac{l_0}{u_0}$. The computational domain has a height $6l_0$ and the particle with diameter $d = 0.25l_0$ is initially positioned in the middle of the channel at a height $4l_0$. The fluid kinematic viscosity ν is set to $0.1(u_0l_0)$ and the solid body density is $\rho_s = 1.25\rho$.

Because the density ratio between the two phases is close to one, the particle quickly reaches its terminal velocity, as evidenced in Fig. 8c. The terminal particle Reynolds number Re_t is 17.4, in good agreement with the values of 17.27 and 17.31 reported for two meshes of increasing resolution

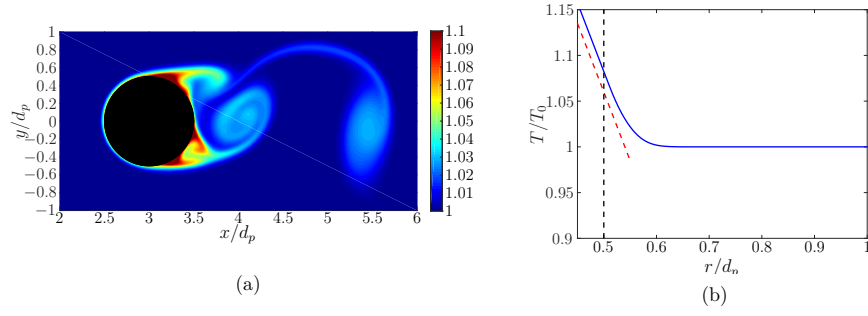


Figure 6: Dimensionless temperature field T/T_0 induced by a heat flux $q = 1.5T_0/d_p$ imposed on the particle surface. (a) Close-up view near the particle (b) Vertical cut across the particle surface (—) and comparison with a line of slope 1.5 (---).

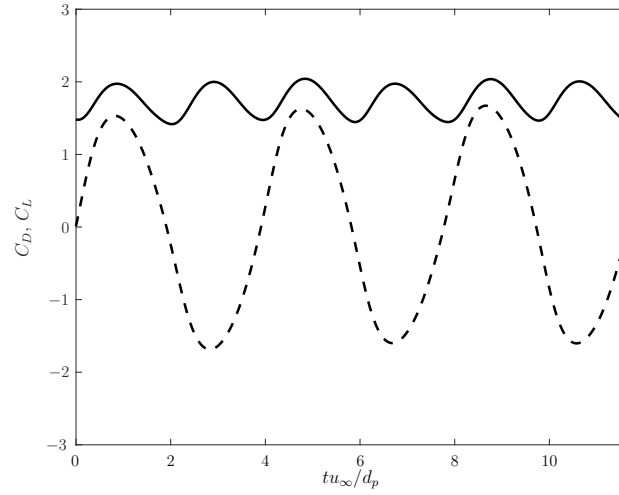


Figure 7: Drag (—) and lift coefficients (---) past a heated cylinder at $Re_p = 1000$.

in [41] and the particle reaching the bottom of the channel around $t = 0.75t_0$

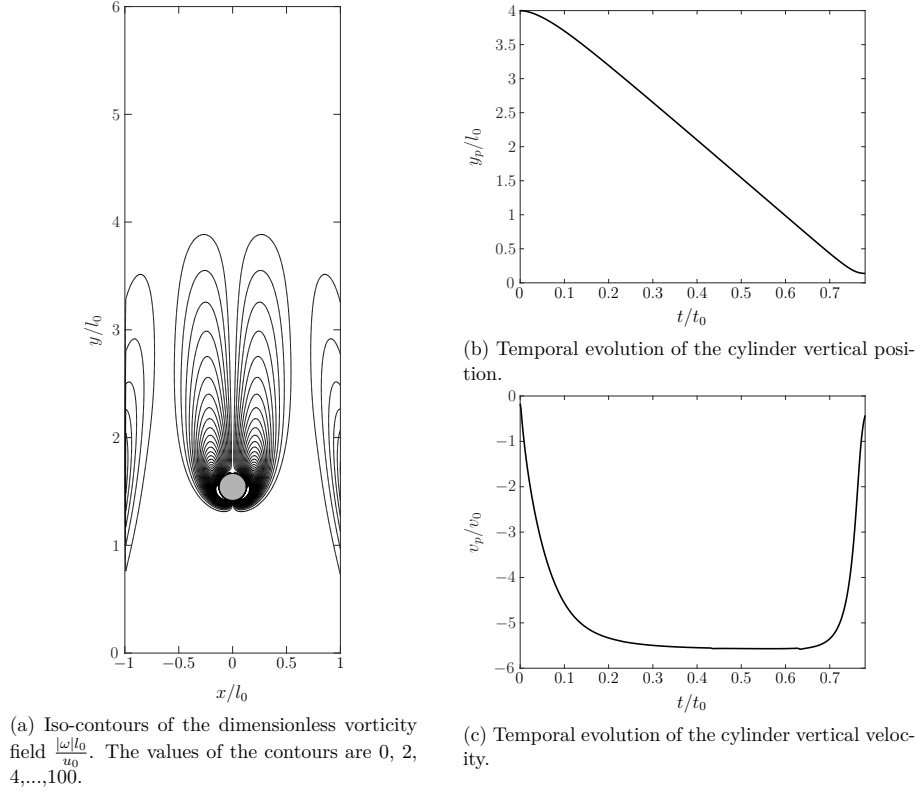


Figure 8: Sedimentation of a cylinder in a channel.

4.3. Drafting-Kissing-Tumbling

The particle-particle interaction part of our method is validated by simulating the sedimentation of two circular particles sedimenting in a channel is simulated, using the results obtained by Glowinski et al. [41] as a reference. The geometrical parameters and reference quantities are identical to those described in the previous section. The solid density is here taken as $\rho_s = 1.5\rho$ and the kinematic viscosity is $\nu = 0.01(u_0 l_0)$. The two particles are initially positioned at $(0, 4.5)l_0$ and $(0, 5)l_0$. The flow field obtained at different dimensionless times is shown in Figure 9. The results obtained match well those obtained from Glowinski et al., with the kissing occurring around $t = 0.15t_0$, the tumbling between 0.15 and $0.2 t_0$ and the final separation of the two particles.

5. Reactive case studies

Depending on the level of approximation and on the comparison of the reaction and mass transfer time scales, different modeling approaches can be considered for the reaction part. In what

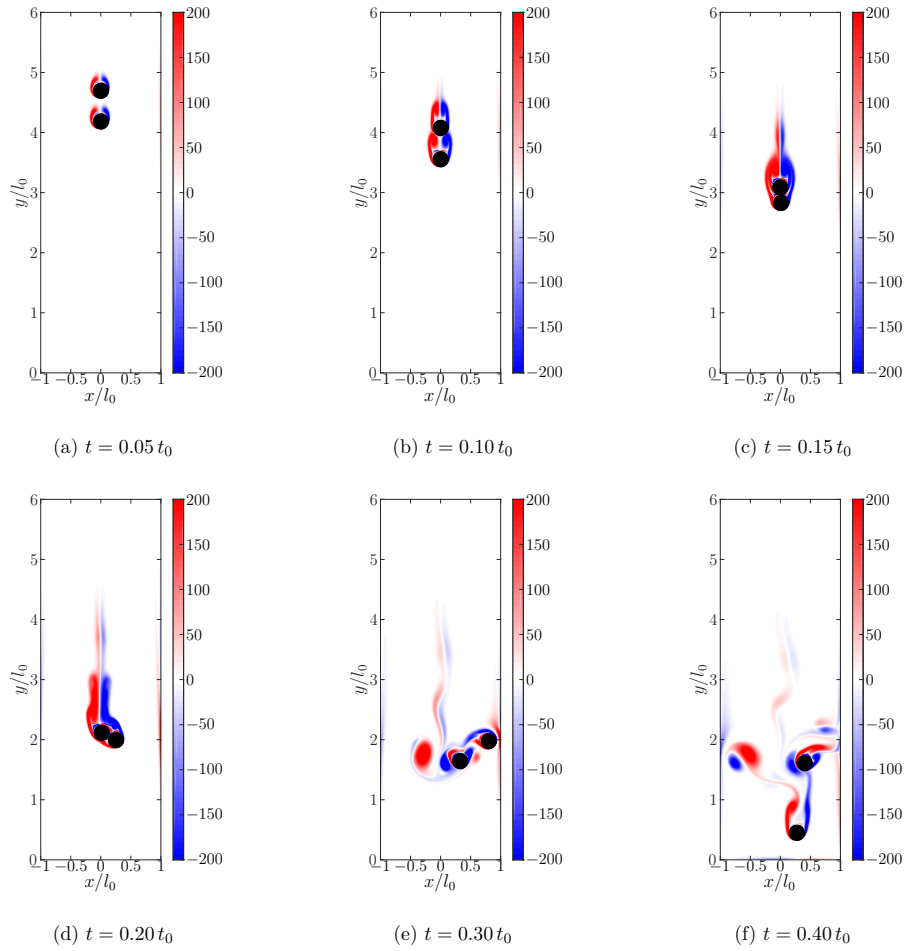


Figure 9: Dimensionless vorticity field $\frac{\omega l_0}{u_0}$ around two circular particles sedimenting in a vertical channel highlighting the drifting-kissing-tumbling phenomenon.

follows, situations with solid-phase finite-rate volume reactions and infinite- or finite-rate surface reactions are addressed. The impact of compressibility on mass and heat transfer is evaluated in the different cases. For all the subsequent simulations, the Schmidt number is fixed as $Sc = \frac{\mu_0}{\rho_0 D} = Pr = 0.7$.

5.1. Intra-particle diffusion-reaction process

The first case considered is that of a finite rate catalytic reaction, with coupled heat and mass transfer between the solid and the fluid phase. The conservation of heat and mass fluxes at the surface of a particle is first verified. Considering a first-order catalytic reaction $A \rightarrow B$, the species transport Eq. (23) is integrated for A with the source terms $w_A = k\rho Y_A$, with k the rate constant with units [1/s]. The effective diffusivity of species in the solid phase is set to one tenth of the fluid-phase diffusivity ($\mathcal{D}_s = 0.1\mathcal{D}$) and the case of a volume Damköhler number $Da_V = \frac{kd_p^2}{\mathcal{D}_s} = 10$ is considered. The mass fraction fields obtained for $Re_p = 40$, $Re_p = 1$ and $Re_p = 0.5$ are shown in Fig. 10a, 10b and 10c respectively. These Reynolds numbers correspond to relevant conditions in fluidized beds, where the slip velocity between the gas and the particle may be very low for small particles at some locations in the bed. The mass fraction profile of species A along a radial cut is extracted in all cases (Fig. 10d) and the slope $\frac{\partial Y_A}{\partial n}$ is evaluated on the particle surface from the fluid and from the solid side. The ratio between these slopes must be the inverse of the diffusivity ratio to satisfy mass flux continuity at the particle surface: $-D\frac{\partial Y_A}{\partial n} = -D_s\frac{\partial Y_{A,s}}{\partial n}$, with $Y_{A,s}$ the mass fraction of A in the solid phase. For a resolution $d_p = 30h$, we obtain a slope ratio of 9.73 (2.7% error), 9.93 (0.7% error) and 9.94 (0.6% error) at $Re_p = 40$, $Re_p = 1$ and $Re_p = 0.5$, respectively. At lower Reynolds number, the conversion across one particle is increased, as a result of the longer effective contact time between the flow carrying the reacting species and the particle. It can also be observed that the intra-particle mass fraction field is nearly perfectly symmetric with respect to the particle center, justifying the classical 1-D radial description used in 1-D or CFD-DEM models. Yet, some symmetry breaking is observed with decreasing Re_p , suggesting a limited validity of this approximation for very low Re_p regimes.

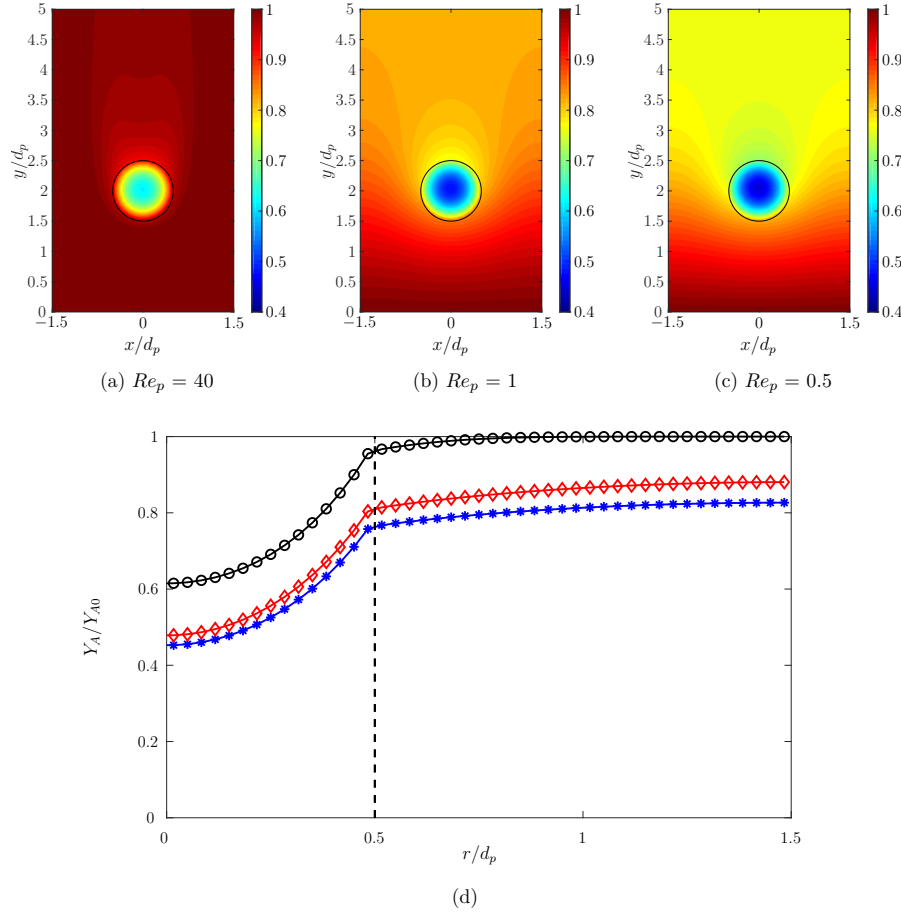


Figure 10: Forced convection coupled to intra-particle diffusion-reaction process; $\mathcal{D}_s = 0.1\mathcal{D}$, $Da_V = 10$, $Sc = 0.7$. (a, b, c) Mass fraction field Y_A/Y_{A0} (d) Mass fraction profile of species A along a horizontal cut through the particle center: $Re_p = 40$ ($\circ$), $Re_p = 1$ ($\diamond$) and $Re_p = 0.5$ ($*$).

5.2. Interfacial mass and heat transfer with infinitely fast reaction

In the case of a very fast irreversible reaction occurring in the solid phase, it can be assumed that the composition of the surface is virtually free of any reactant species. For the model reaction $A \longrightarrow B$, this amounts to impose $Y_A = 0$ and $Y_B = 1$ on the particle surface. It follows that the observed consumption rate of A over a particle, R_A in [kg/s], is determined by the interfacial transfer of A : $R_A = \dot{m}_{A,f \rightarrow s}$. The interfacial flux $\dot{m}_{A,f \rightarrow s}$ is obtained by integrating the penalization

term over the volume of the particle:

$$\begin{aligned}
 \dot{m}_{A,f \rightarrow s} &= \oint_{\partial\Omega_s} \mathbf{j}_A \cdot \hat{\mathbf{n}} dS = \oint_{\partial\Omega_s} (\rho Y_k \mathbf{v}_k) \cdot \hat{\mathbf{n}} dS \\
 &= - \int_{\Omega_s} \nabla \cdot (\rho Y_k \mathbf{v}_k) dV \\
 &= \int_{\Omega_s} \rho \underbrace{\frac{DY_A}{Dt}}_{=0} dV + \int_{\Omega_s} \chi \left(\rho \frac{(Y_k - Y_{k,s})}{\Delta\tau} \right) dV \\
 &= \int_{\Omega_s} \chi \left(\rho \frac{(Y_k - Y_{k,s})}{\Delta\tau} \right) dV.
 \end{aligned} \tag{44}$$

where the first term on the right-hand side vanishes because of the fixed surface composition.

If it is further assumed that the solid phase thermal conductivity is sufficiently large that it uniformizes its temperature in a time much smaller than the characteristic time of the fluid-solid heat transfer. The temperature of the solid phase is therefore considered as uniform and a global heat balance can be solved:

$$m_s c_{p,s} \dot{T}_s = Q_r + Q_{f \rightarrow s}, \tag{45}$$

with Q_r , the total heating rate (in [W]) induced by the reaction and computed as

$$Q_r = \sum_{k=1}^{N_s} R_k h_k, \tag{46}$$

and $Q_{f \rightarrow s}$, the interfacial heat flux. The latter is obtained after integration of the penalization term on the energy equation:

$$\begin{aligned}
 Q_{f \rightarrow s} &= \oint_{\partial\Omega_s} \mathbf{q} \cdot \hat{\mathbf{n}} dS = \oint_{\partial\Omega_s} \kappa \nabla T \cdot (-\hat{\mathbf{n}}) dS \\
 &= \int_{\Omega_s} \nabla \cdot (\kappa \nabla T) dV \\
 &= \int_{\Omega_s} \rho c_p \frac{DT}{Dt} dV + \int_{\Omega_s} \chi \left(\rho c_p \frac{(T - T_s)}{\Delta\tau} \right) dV \\
 &= \dot{T}_s \int_{\Omega_s} \rho c_p dV + \int_{\Omega_s} \chi \left(\rho c_p \frac{(T - T_s)}{\Delta\tau} \right) dV.
 \end{aligned} \tag{47}$$

The combination of Eqs. (45) and (47) gives

$$\dot{T}_s = \frac{\left(Q_r + \int_{\Omega_s} \chi \rho c_p \frac{(T - T_s)}{\Delta\tau} dV \right)}{\left(m_s c_{p,s} - \int_{\Omega_s} \rho c_p dV \right)}. \tag{48}$$

The value of T_s at the next time step is then used as the new Dirichlet condition in the penalization term of Eq. (15).

Considering an exothermic reaction, the increase of the particle temperature, T_s , with time is

plotted in Fig. 11a for the enthalpies of formation $h_A = 0.5(c_{p,0}T_0)$, $h_B = 0$. The solid density ρ_s and specific heat $c_{p,s}$ are set equal to $10\rho_0$ and $c_{p,0}$, respectively. It can be observed that T_s increases slower in the weakly compressible case. Because the intrinsic reaction rate is considered infinite, this can be attributed to the reduced mass transfer rate of reactant A from the fluid phase, as evidenced in Fig. 11b, hence reducing the consumption rate of A and the heat generation in the body of the particle. The heat transfer from the fluid phase is subsequently lowered, as a result of the decreased driving force $(T_s - T_0)$.

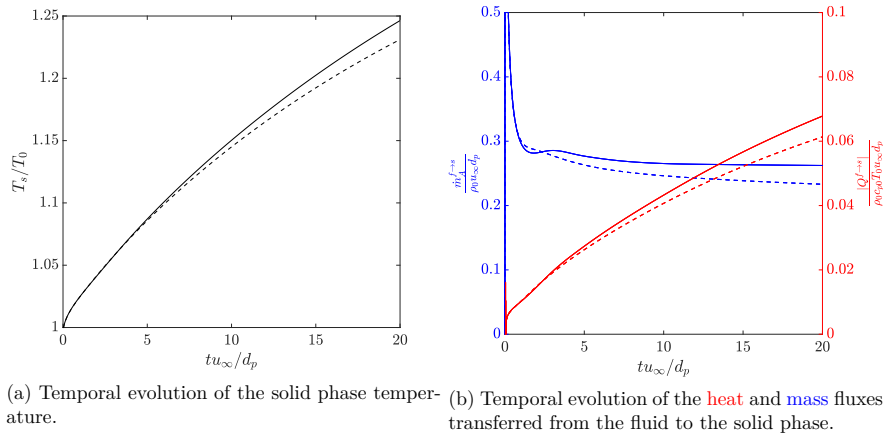


Figure 11: Infinitely fast and irreversible reaction $A \longrightarrow B$ with uniform solid phase temperature: incompressible (solid line) and weakly compressible (dashed line) cases. $Re_p = 40$, $Sc = Pr = 0.7$; $h_A = 0.5(c_{p,0}T_0)$, $h_B = 0$; $\rho_s = 10\rho_0$, $c_{p,s} = c_{p,0}$.

5.3. Interfacial mass transfer with finite rate surface reaction

An interesting application of the extension of the penalization method to Neumann- and Robin-type boundary conditions is the case of a surface reaction with finite rate chemistry. Considering, as in [42], an irreversible first order reaction in the absence of accumulation on the surface, the diffusion flux of the reacting species A at the solid surface balances exactly its rate of consumption:

$$\mathbf{j}_A \cdot \hat{\mathbf{n}} = -\rho \mathcal{D} \frac{\partial Y_A}{\partial n} = k_s \rho Y_A, \quad (49)$$

where k_s is the surface rate constant, with units [m/s] and the unit normal vector $\hat{\mathbf{n}}$ is pointing towards the interior of the solid phase.

Eq. (49) constitutes a Robin-type boundary condition on the particle surface for the species transport equation in the fluid. Indeed, it can be recast as

$$Da_s Y_A + d_p \frac{\partial Y_A}{\partial n} = 0, \quad (50)$$

with $Da_S = \frac{k_s d_p}{D}$, the Damköhler number based on the surface reaction rate and the fluid diffusivity. Following the CBVP approach detailed in Section 2.2.2, the species transport Eq. (21) for a surface reaction is modified as

$$\frac{\partial Y_k}{\partial t} = (1 - \chi) \left(-\mathbf{u} \cdot \nabla Y_k + \frac{1}{\rho} \nabla \cdot \left(\frac{\rho D}{\bar{W}} \nabla (Y_k \bar{W}) \right) \right) - \frac{\chi}{\eta_c} \left(\left(\frac{Da_s}{d_p} \right) Y_A + \hat{\mathbf{n}} \cdot \nabla Y_k \right). \quad (51)$$

A drawback of the CBVP method for the implementation of Neumann- and Robin-type boundary conditions is the non-straightforward implicit integration of the penalization term. In contrast to the case where a Dirichlet boundary condition is prescribed, the penalization term is no longer local as it involves spatial derivatives of the solution. Hence, an explicit formulation of the penalization term must be used, making the constraint on the time step much stronger to guarantee an acceptable accuracy of the solution in the vicinity of the solid boundary. Typically, we found that the condition $\eta_c u_\infty \gtrsim \frac{u_\infty \Delta t}{h}$ had to be satisfied to ensure stability.

The generic surface reactions $A \longrightarrow B$ and $A \longrightarrow 2B$ are investigated in a systematic manner. The penalization parameter η_c in Eq. (51) is fixed to $\eta_c = 0.1/u_\infty$. Fig. 12 shows the resulting mass fraction field of species A in the case of the equimolar surface reaction $A \longrightarrow B$ and for $Da_S = 1$. The flow is simulated for different values of Da_S and the mass fraction profiles of A in the wake of the cylinder (through the particle center), are reported in Fig. 13a. As expected, with increasing Damköhler number, the effect of the surface reaction is more pronounced and the depletion of species A in the wake is more important. The case $Da_S = \infty$ corresponds to the situation of an infinitely fast reaction with zero mass fraction on the particle surface, leading to the Dirichlet boundary condition $Y_A = 0$. On the other hand, when $Da_S = 0$, the situation corresponds to an extremely fast diffusion process (or slow reaction) such that the species concentration gradients induced by the reaction are instantaneously smeared out, leading to a no-flux Neumann boundary condition: $\frac{\partial Y_A}{\partial n} = 0$.

For the reaction $A \longrightarrow 2B$, Fig. 13a also shows the effect of the molecular weight decrease on the consumption rate of reactant A . At low Da_S , the depletion of the reactant A is slightly more pronounced when the reaction is accompanied with volume expansion ($A \longrightarrow 2B$) while at higher Da_S , when diffusion becomes the rate-limiting process, the trend reverses and the volume expansion results in a lower conversion of A than the equimolar case $A \longrightarrow B$.

Fig. 13b shows the mass fraction profile perpendicular to the flow (vertical cut through the particle center in Fig. 12) obtained inside and outside the particle. The hyperbolic region where the characteristics are propagated and the diffusive region which acts as a support to the solution are clearly evidenced.

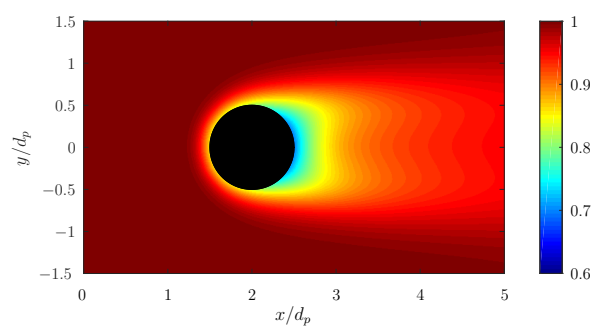
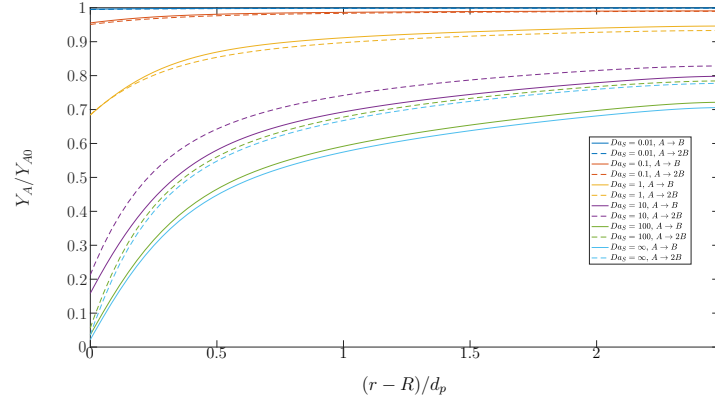
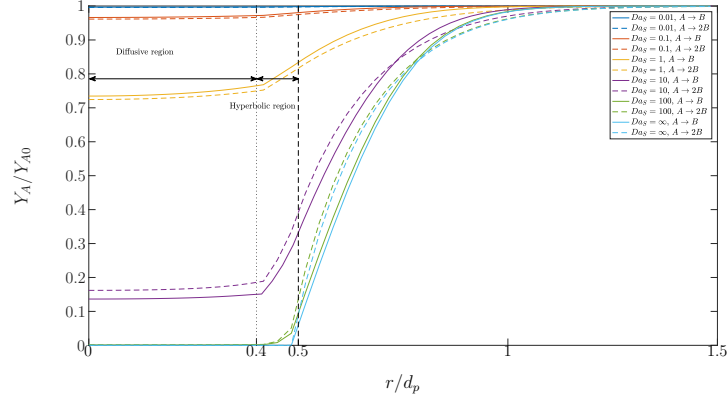


Figure 12: Iso-contours of Y_A/Y_{A0} for a surface reaction $A \longrightarrow B$ and with $Da_S = 1$, $Re_p = 40$, $Sc = 0.7$.



(a) Mass fraction profile of species A in the wake of the particle (horizontal cut through the particle center).



(b) Mass fraction profile of species A along a vertical cut through the particle center with finite-rate surface reaction.

Figure 13: Surface reactions $A \longrightarrow B$ and $A \longrightarrow 2B$ at different Da_S ; $Re_p = 40$, $Sc = 0.7$.

6. Conclusion

In this work, a new combination of the weakly compressible approximation and the Brinkman penalization method was developed. The method was validated against literature benchmarks at different particle Reynolds numbers, in static and moving configurations. Different situations encountered in reacting gas-solid flows were subsequently addressed. Using the classical formulation of the penalization method for Dirichlet-type boundary conditions, we performed a set of numerical experiments with increasing values for the solid phase temperature, highlighting the decrease of the heat transfer rate and the increase of the drag coefficient relatively to the incompressible case. The situation where the external flow is coupled to an intra-particle diffusion-reaction process was simulated for different particle Reynolds numbers corresponding to relevant conditions in industrial fluidized beds. The reduction of the slip velocity based Reynolds number induced by the fluidization regime was shown to improve the usage of the catalytic phase, and hence the conversion. It appeared that the classically used 1-D radial approximation for the intra-particle species profiles was fairly well verified down to $Re_p = 0.5$. Yet, the asymmetry inside the particle increases with decreasing Re_p and it can be expected that at locations in the bed where the slip velocity is very low, this approximation will be less valid. The case of an infinitely fast catalytic reaction with subsequent heat release in the solid phase and considering a high solid thermal conductivity was then studied. It showed a reduced mass transfer rate from the fluid to the solid phase because of the reduced density of the fluid surrounding the particle, resulting in a slower increase of the solid phase temperature. The imposition of Neumann- and Robin-type boundary conditions was performed using the characteristic based volume penalization (CBVP) method developed by Brown-Dymkoski et al. [22]. It allowed to treat the interesting case of finite-rate surface reactions. It was shown that the decrease of the fluid density induced by composition modifications tends to reduce the conversion of the reactant in the wake of the particle when diffusion becomes the rate-limiting phenomenon. This effect would also appear in cases where the fluid goes through an array of particles, like in fixed bed reactors. Future work will be dedicated to the efficient three-dimensional implementation of the method so as to build new meso-scale models for static (fixed bed) and moving (fluidized bed) configurations.

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