

THE DYNAMICS OF SPHERES IN OSCILLATORY FLUID FLOWS

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Abstract

In this thesis we present an experimental and numerical study of the interactions between rigid spherical particles under horizontal vibration in a liquid-filled cell.

First, we introduce the computational model which is used for simulating a system of interacting spheres in an oscillatory flow, at finite Reynolds numbers in the range 3-120. The model includes the solution to the Navier-Stokes equations for the fluid, the particle-fluid coupling force and the treatment of the collisions between the spheres themselves.

We begin our study by looking at the details of a single isolated oscillating sphere. When a solid sphere is oscillating in a fluid at intermediate Reynolds numbers, there is a non-zero time averaged flow, called *steady streaming* generated around it. We discuss the structure of the steady streaming flow near and far from the sphere, as reported in various analytic, experimental and numerical studies. Our own computational model for the fluid and the spheres can capture this behaviour reasonably well and reproduce the principal features of the experimentally-observed and theoretically-predicted behaviour.

Through experiments and simulations we then investigate the interactions for two stainless steel spheres oscillating in a finite box. We find that two spheres under horizontal vibration align at right angles to the oscillation axis and sit with a well-defined gap between them. We then carry out experiments measuring the equilibrium gap between the two particles for various vibratory conditions and three different fluid viscosities. Two distinct scaling regimes have been identified for the gap. We then perform simulations for the same system and find that the structure of the fluid field around the pair of spheres also differs between the two scaling regimes and we see a transition from one flow field to the other with an increase of the amplitude of oscillation. Moreover, for a given set of parameters,

the structure of the outer streaming flow for the pair is found to resemble that of a single sphere.

We then proceed onto the study of a more complex system: the interactions between a large number of spheres under horizontal vibration which evolve to form long chains; a pattern already observed experimentally. Through computer simulations, we study in detail all the steps of the evolution of the system, which goes from an initially spatially-dispersed configuration of spheres to a regular chain pattern spanning the available space in the box. We demonstrate that the spheres align locally across the flow, due to the circulation of the steady streaming flows and stabilise when they form full chains across the width of the container. The interaction between full chains is also investigated for longer time-scales and we can identify a long-ranged repulsion between neighbouring chains.

We finally address issues relating to the effects of friction, the size of the container and the interactions between two spheres of unequal size.

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Publications

The following papers have been published as a result of this research:

1. D. Klotsa and M. R. Swift and R. M. Bowley and P. J. King. *Interaction of spheres in oscillatory fluid flows*, Physical Review E, **76**, 056314 (2007).
2. D. Klotsa and M. R. Swift and R. M. Bowley and P. J. King. *Chain formation of spheres in oscillatory fluid flows*, Physical Review E, **79**, 021302 (2009).
3. M. R. Swift, D. Klotsa , H. S. Wright, R. M. Bowley and P. J. King. *The dynamics of spheres in oscillatory fluid flows*, Powders and Grains (2009).

The following poster has been presented at a conference:

1. D. Klotsa, M. R. Swift, R. M. Bowley and P.J. King. *Interaction of spheres in oscillatory fluid flows*, Presented to the Satellite conference of Statphys 23, *Statics and Dynamics of granular media and colloidal suspensions*, July 2007 Napoli, Italy.

The following presentations have been given:

1. D. Klotsa. *Simulating granular dynamics*, Presented to the Nottingham High Performance Computing User Meeting (January 2006), University of Nottingham, Nottingham, U.K.
2. D. Klotsa. *Pattern formation in oscillatory fluid flows*, Informal seminar (September 2008), Condensed matter theory group, the Rudolf Peierls Centre for Theoretical Physics, University of Oxford, U.K.
3. D. Klotsa. *Structure formations of spheres in oscillatory fluid flows*, Invited seminar (May 2009), Theoretical Physics Group, University of Warwick, U.K.

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Chapter 1

Introduction

The present thesis describes the behaviour of fluid-immersed dilute granular systems subjected to horizontal vibration. In this introductory chapter we give an overview of the field of Granular Physics focussing on granular systems immersed in fluids. We then describe in detail two experiments by Wunenburger *et al.* (2002) and by Voth *et al.* (2002) which demonstrate the formation of ordered structures in particle-laden flows. The mechanism responsible for these structures was unknown and became the motivation for our studies. At the end of the Chapter, we give an outline of the rest of the thesis.

1.1 Granular matter

Granular matter refers to systems which consist of a large number of discrete, solid, macroscopic particles. Everyday examples include sand, coffee, sugar, pharmaceuticals, powders, gravel and coal. All the industrial processes using these materials, from storing and transporting, to mixing and separating them require an understanding of their properties (Jaeger *et al.* 1996). Geological processes too involve naturally occurring granular systems, such as sand dunes, snow avalanches and volcanic ash flows (Dartville 2004). In terms of the grain particle size, there is no upper limitation. An example of large granular systems are rubble-pile asteroids consisting of chunks of rock held together by gravity (Sharma *et al.* 2009, Spahn *et al.* 2000).

Despite their prevalence in nature and industry, and their apparent simplicity,

granular materials exhibit a rich phenomenology and complex behaviour which is still not fully understood (Sun 2009). Let us consider the simple case of sand. We can make a sandpile which remains static and behaves as a collection of solid particles if the slope of the pile is below a certain threshold, called the angle of repose. Beyond the angle of repose, the top layer of the sand particles start to avalanche and we observe motion that superficially resembles that of a fluid. This simple sandpile has been used as a model complex system of self-organised criticality (Bak *et al.* 1987, Mehta and Barker 1994).

Granular materials have two important characteristics: the grains are not affected by thermal fluctuations and the interactions between the grains dissipate energy due to the inelasticity of the collisions between them. These two characteristics imply that equilibrium assumptions from statistical mechanics do not necessarily apply. For example, shaking a granular material which consists of two types of grains can lead to separation of the two species rather than mixing (Kudrolli 2004), which would be expected if “entropy” were to be maximised. When a granular bed is given a large energy input, such as by shaking or rotating, the substance flows like a fluid. If the energy input is even larger and the particle density is low then the substance resembles a gas in Brownian motion. Continuum theories have been developed analogous to the Navier-Stokes equations in order to describe granular hydrodynamics and concepts from the Kinetic Theory of gases have been employed to describe granular gases (Goldhirsch 2003). However, there is no consistent theory to describe their physical properties which, as just described, are observed to superficially resemble solids, fluids or gases depending on the energy input and the number of grains involved. There are many reviews which summarise the properties, the theoretical concepts and developments of granular materials (Ausloos *et al.* 2005, Jaeger *et al.* 1996).

A large number of granular phenomena occur as a result of the interaction between the grains and the fluid in which they are immersed. The presence of fluid significantly complicates the granular system, but also gives rise to very interesting phenomena which range from simple sedimentation (Ramaswamy 2001), segregation (Burtally *et al.* 2002) to bifurcation (Mullin *et al.* 2009) and chaos (Pine *et al.* 2005). Sand dunes and ripples for example are formed as a result of

the interaction between the strong winds in the desert and the grains of sand and exhibit very interesting properties (Bagnold 1954) which are still actively studied (Schwammle and Herrmann 2003, Parteli *et al.* 2007). Another example is the convection and Faraday tilting of vertically-shaken, dense granular beds which is driven by the presence of air (Faraday 1931, Milburn *et al.* 2005).

1.2 Pattern formation in fluid-granular systems

Recently there has been a lot of interest in the collective behaviour and pattern formation in granular matter (Aranson and Tsimring 2006), which can be enhanced by the presence of a fluid. In particular, ordered structures have been observed to form between spherical particles in oscillatory fluid flows (Wunenburger *et al.* 2002, Voth *et al.* 2002, Thomas and Gollub 2004). We shall describe in detail two experiments which acted as the motivation for the research carried out in this thesis.

Wunenburger *et al.* (2002) reported experiments in which small metal spheres were placed in a water-filled cell which was undergoing horizontal, sinusoidal vibration. The dimensions of the shallow cell were $100 \times 100 \times 10$ mm, the orientation of which is shown in Fig. 1.1 (a). The polydisperse mixture of roughly spherical bronze particles had diameters d in the range $d=280\text{-}630\mu\text{m}$, the frequency range was $f=10\text{-}20\text{Hz}$ and the driving amplitude was $A=0.7\text{-}3.5\text{mm}$. Because the spheres were not neutrally buoyant they would sink to the bottom surface and oscillate with respect to the fluid once the vibration was switched on. If we define the Reynolds number to be $\text{Re}=2\pi f d A/\nu$, where ν is the kinematic viscosity of the liquid, we get an estimate for the Reynolds number range in Wunenburger *et al.*'s experiments between 1-280.

The spheres were initially clustered together in the middle of the cell, as shown in Fig. 1.1 (b). As soon as the vibration was switched on, the spheres were observed to form equally spaced chains, each oriented perpendicular to the direction of oscillation, a top view is shown in Fig. 1.1 (c). Wunenburger *et al.* (2002) found that the periodic pattern of chains shrank and expanded, in other words that the distance *between* the chains increased and decreased depending on the

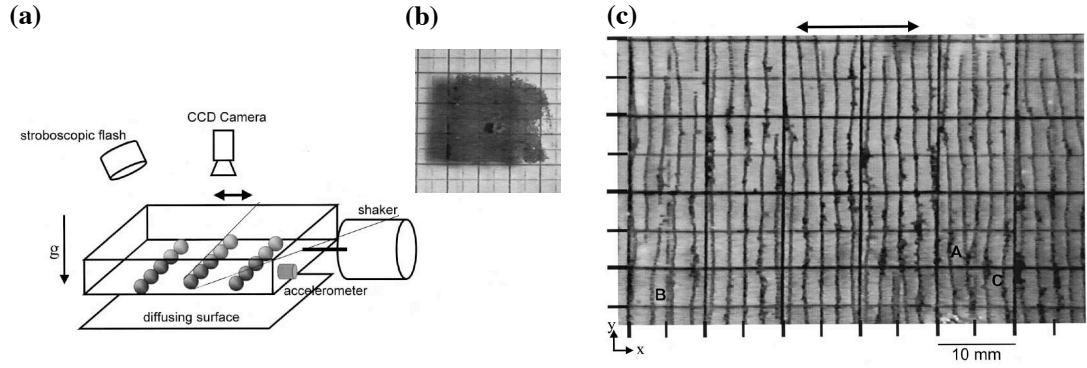


Fig. 1.1: (a) The experimental arrangement used by Wunenburger *et al.* (2002). (b) Top view of the initial configuration of the particles which is a clump in the middle of the cell. (c) Top view of the chains of particles formed in water, perpendicular to the vibration axis (horizontal) as indicated by the double-headed line. All images are taken from (Wunenburger *et al.* 2002).

vibratory conditions, although the initial configuration had the particles always clustered together in the middle. The exact mechanism behind the formation of the pattern was not fully understood and was left as an open question.

Using a different experimental arrangement, shown in Fig. 1.2 (a), Voth *et al.* (2002) observed the clusters and hexagonal lattices of lead spheres, shown in Fig. 1.2 (b). They used a vertically vibrated cell filled with a more viscous, glycerol/water mixture and the spheres were stainless steel, 0.8mm in diameter. The Reynolds number range for Voth *et al.*'s experiments was between 2-10. The spheres would bounce on the vibrating base of the cell under the influence of gravity and fluid-induced interactions in the plane perpendicular to the axis of vibration made the spheres cluster together and form various structures. A top view is shown in Fig. 1.2(b). We can identify an attraction and a repulsion between the spheres in that plane as they cluster but sit a distance apart. Thomas and Gollub (2004) investigated the same system theoretically and discussed the chaotic fluctuations in the positions of the spheres after the clusters were formed. After varying the number of particles, they concluded that the inter-particle forces are not simply pairwise additive but that there are nonlinear hydrodynamic interactions between the spheres.

It may be that these two systems are governed by the same mechanisms. In both experiments there is vibration of macroscopic dense spheres which form structures perpendicular to the direction of oscillation. More specifically, in Wunenburger *et al.* (2002) there is an attraction between the spheres which

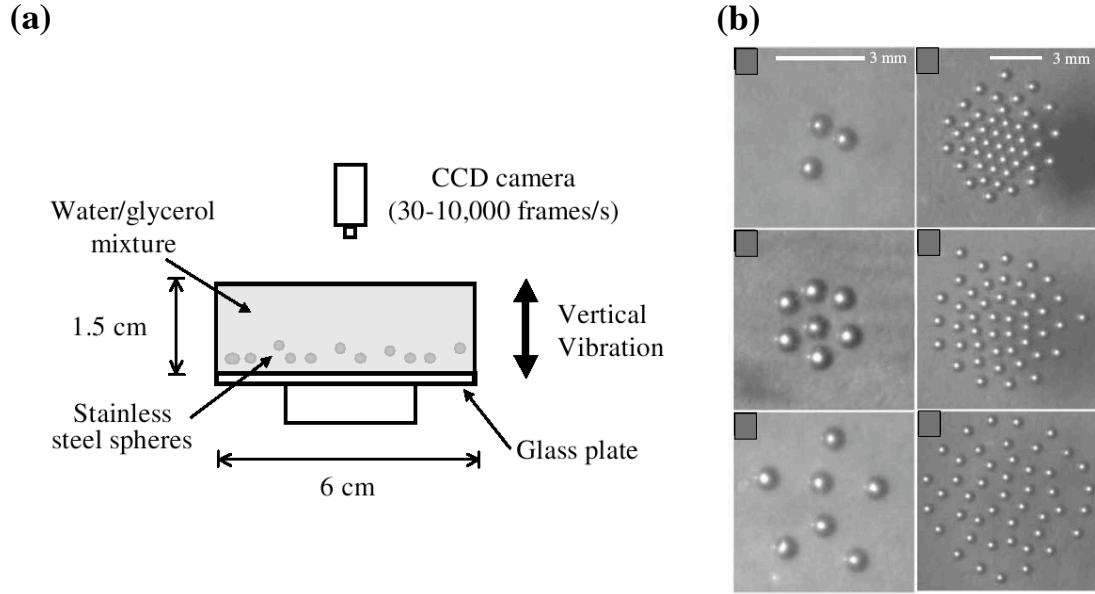


Fig. 1.2: (a) The experimental arrangement used by Voth *et al.* (2002). (b) Top view of the lattice structures formed by steel spheres in a viscous fluid in a vertically-vibrated container. The interactions are in a plane perpendicular to the vibration axis which is in and out of the page. All images are taken from (Voth *et al.* 2002).

leads to the formation of a chain oriented perpendicular to the axis of oscillation. In Voth *et al.* (2002) there is an attraction and a repulsion on the plane perpendicular to the oscillation which leads to the formation of lattice structures. Furthermore, the Reynolds number ranges in both experiments lie in the intermediate regime where the flows are both viscous and inertial. In their explanation of these phenomena both groups discussed the existence of a non-zero, time-averaged flow which exists at non-zero Reynolds numbers in oscillatory flows, called *steady streaming* (Riley 1966, Riley 2001). However, experimentally, three-dimensional fluid flows are difficult to track and visualise and direct observation or measurement of flows was beyond the scope of their studies.

To sum up, there is the indication and suggestion that steady streaming is the mechanism for the attraction between spheres but there is no explanation for the repulsion. A number of questions remain open:

- In the plane perpendicular to the axis of oscillation, why is there only attraction between the spheres in Wunenburger's experiments whilst in Voth's experiments there is an attraction and a repulsion?
- Is there evidence for the suggestion that the source of attraction is steady

streaming?

- What is the source of the repulsion in Voth's experiments?
- What is the interaction between just two spheres in an oscillatory flow?
- What is the mechanism behind the chain formation?
- What is the interaction between chains?

In order to answer these questions and understand the mechanism and details behind the formation of the structures observed by Wunenburger *et al.* (2002) and Voth *et al.* (2002) we have proceeded as follows. We use a horizontal arrangement similar to that of Wunenburger *et al.* (2002) but with monodisperse steel spheres of slightly bigger size, 1mm diameter. We vary the viscosity of the liquid and see how that affects the system. Note that the solution in Wunenburger *et al.* (2002) was water whereas in Voth *et al.* (2002) the viscosity of the liquid was eight times that of water. We start by studying the interaction between two spheres aiming to clarify why Wunenburger *et al.* (2002) observed only attraction and Voth *et al.* (2002) both an attraction and a repulsion. By adding spheres into the system we then investigate the formation of a chain through simulations. Finally, the goal is to identify the interaction between neighbouring chains and understand the behaviour of the pattern as a whole.

1.3 Thesis outline

The plan of the thesis is the following.

Chapter 2 introduces the governing equations and a number of computational approaches which can be used to model particles-laden flows. A more detailed description of the model which has been used throughout this thesis is given. More specifically, the fluid is described by the three-dimensional Navier-Stokes equations which are numerically solved using the projection method (Chorin 1968, Temam 1969). The coupling between the particles and the fluid is achieved through a particle-template model (Höfler and Schwarzer 2000). The collisions between the particles themselves and between the particles and the walls of the

container are simulated using molecular dynamics techniques (Allen and Tildesley 2000). We have included a validation for each of the models.

Chapter 3 focuses specifically on oscillatory systems. An explanation and literature review of studies relating to steady streaming flow is given. The governing equations and characteristic dimensionless parameters, such as the Reynolds number, are defined. The computational model is validated for our purposes in oscillatory flows, at intermediate Reynolds numbers against experiments and numerical methods for a single sphere. We then study the influence of flat boundaries, such as those of a container. In particular we have looked at the flow field for an oscillating sphere near a boundary and have measured the force on it due to the presence of the boundary as a function of distance from the boundary. The exact geometry of the systems which shall be used in the rest of the thesis is presented.

Chapter 4 describes a series of experiments for two spheres in a finite fluid-filled container under horizontal vibration. We find that the two spheres attract each other, align perpendicular to the axis of oscillation and sit at a well-defined distance. We have measured the gap between the spheres for various vibratory conditions, fluid viscosities and sphere diameters and have discovered two scaling regimes, depending on the amplitude of oscillation (Klotsa *et al.* 2007).

In **Chapter 5** we carry out simulations for the two-sphere system used in the experiments of Chapter 4. Measuring the gaps between the spheres we achieve reasonable agreement with the experiments, identifying two scaling regimes depending on the amplitude. We then use our simulations to investigate in depth the fluid fields and measure the forces between the two spheres when they are oscillating at equilibrium. We find that the time-averaged fluid field around a pair of spheres at equilibrium resembles at long distances that of a single sphere. The far fluid field is responsible for the attractive force between the two spheres, whereas the fluid field in the gap between the spheres provides the repulsive force. Moreover, we discover a transition in the structure of the fluid field around the pair when we move from one regime to the other (Klotsa *et al.* 2007).

In **Chapter 6** we perform experiments and simulations for a system of sixty-four spheres undergoing horizontal vibration and investigate the formation and

evolution of chains from an initially-dispersed configuration. We use our simulations in order to study in detail each step of this process by looking at the formation of a pair, a short chain, a chain attached to one wall and then a full chain which spans the width of the cell. Finally, we discuss the interactions between chains and the stability of the pattern. (Klotsa *et al.* 2009).

Chapter 7 reviews the research carried out in this thesis with a summary of each chapter, the general conclusions that can be drawn as well as possible improvements, open questions and new pathways leading to future research.

Chapter 2

Computational Model

In this chapter, after a brief introduction into Computational Fluid Dynamics (CFD), we shall explain in detail the computational methods we have used in order to study fluid-immersed oscillatory granular systems. More specifically, we first describe the model for the fluid, which is a numerical solution of the Navier-Stokes equations using the projection method (Höfler and Schwarzer 2000). The coupling between the particles and the fluid is achieved through a simplified version of the particle-template model and is described next. Finally, for the collisions between the spheres we have used Molecular Dynamics (MD) methods which are well-understood and commonly-used to simulate granular beds. We end with a short discussion and flow-diagram which illustrates the order in which the simulation runs.

2.1 Introduction

Computer simulation is a very valuable tool in physics. In limits where analytic solutions are unattainable and experiments are very elaborate, computer simulations provide a clean method to investigate problems. Our aim is to model a system that consists of macroscopic spheres which are free to move and to collide with one another in a fluid.

Computational Fluid Dynamics (CFD) is the area of fluid dynamics which uses numerical methods and simulations to solve and analyse problems which involve fluid flows. As the range of phenomena which occur in fluid flows is immense, so

is the number of ways to model them computationally. As a result, these ways of modelling vary greatly from one another. CFD is a field which covers a broad spectrum from simple, basic algorithms to extremely sophisticated, specialised commercial tools. As Riley put it in Drazin and Riley (2006), the development of Computational Fluid Dynamics caused a shift in the emphasis from finding exact solutions of approximate problems to finding approximate solutions of exact problems.

One way to categorise CFD methods is based on whether the fluid is described as a collection of fluid molecules/particles, or as a continuum. A molecular description for the fluid is not plausible when macroscopic objects are also present because the length and time scales of the fluid molecules and the solid macroscopic particles are too different from one another. There are various *mesoscopic* approximations which use coarse-graining schemes to model the vast number of fluid molecules such as: the Lattice-Boltzmann Method (LBM) (Ladd and Verberg 2001), Dissipative Particle Dynamics (DPD) (Hoogerbrugge and Koelman 1992) and, Smoothed Particle Hydrodynamics (SPH) (Monaghan 2005).

In the *continuum* approximation for the fluid, which has been used throughout this thesis, the fluid dynamics is governed by the Navier-Stokes equations, which are a set of nonlinear partial differential equations. There are many ways to numerically solve the Navier-Stokes equations. Most of them use discretisation techniques, which means that the spatial domain is divided into unit cells forming a mesh. A suitable algorithm is then used to solve the equations in time. Finite-Difference (FDM), Finite-Volume (FVM), Finite-Element (FEM) and Compact Finite-Difference Methods (CFDM) are some common examples (Ferziger and Peric 2002). There are also mesh-free techniques used to solve partial differential equations such as Spectral Methods which make use of Fourier Transforms and Chebychev polynomials (Peyret 2002). Note that the mesoscopic methods mentioned earlier, SPH and DPD are also mesh-free. In the high Reynolds number limit, more complex methods have been developed to describe turbulent flow, such as the Large Eddy Simulation (LES) or the Reynolds-averaged Navier-Stokes equations (RANS).

2.2 Fluid model

2.2.1 Navier-Stokes Equations

In the continuum approximation the fluid is described through its macroscopic properties of density, viscosity, pressure and velocity, without worrying about the individual motion and collisions of particles on a microscopic level. Mathematically, this is expressed through the Navier-Stokes equations for conservation of momentum and mass, which in general for a Newtonian fluid are given by

$$\rho \frac{D\mathbf{u}}{Dt} = \mathbf{f} + \nabla \cdot \sigma \quad (2.1)$$

and

$$\frac{1}{\rho} \frac{D\rho}{Dt} + \nabla \cdot \mathbf{u} = 0 \quad (2.2)$$

respectively, where $\rho(\mathbf{x}, t)$ is the fluid density, $\mathbf{u}(\mathbf{x}, t)$ the fluid velocity, $\mathbf{f}$ is a system force and σ is the stress tensor of the fluid at position $\mathbf{x}$ and time t . The operator D/Dt is called the convective derivative and is equal to

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla \quad (2.3)$$

The Navier-Stokes equations (2.1) and (2.2) are nonlinear in $\mathbf{u}$ and have therefore limited analytic solutions. Approximate solutions exist either in an asymptotic or in a numerical sense. We shall explain each term in Eq.(2.1) in more detail and derive the exact form in which the Navier-Stokes equations are used in the systems we are investigating.

The symmetric stress tensor σ_{ij} has normal stress elements σ and shear stress elements τ_{ij}

$$\sigma_{ij} = \begin{pmatrix} \sigma_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \sigma_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \sigma_{zz} \end{pmatrix} \quad (2.4)$$

and can be split into two terms

$$\sigma_{ij} = - \begin{pmatrix} P & 0 & 0 \\ 0 & P & 0 \\ 0 & 0 & P \end{pmatrix} + \begin{pmatrix} \sigma_{xx} + P & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \sigma_{yy} + P & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \sigma_{zz} + P \end{pmatrix},$$

$$\sigma_{ij} = -PI + \mathbb{T}. \quad (2.5)$$

where I is the 3×3 identity matrix and P is the pressure. Substituting σ in Eq.(2.1) gives

$$\rho \frac{D\mathbf{v}}{Dt} = \mathbf{f} - \nabla P + \nabla \cdot \mathbb{T}. \quad (2.6)$$

The pressure gradient ∇P arises from normal stresses. The stress derivative term $\nabla \cdot \mathbb{T}$ conventionally describes viscous forces and usually requires that an assumption on the viscous behaviour of the fluid is made. For incompressible, Newtonian fluids $\nabla \cdot \mathbb{T} = \eta \nabla^2 \mathbf{v}$, where η is the dynamic viscosity. Under the assumption of incompressibility the fluid density ρ is constant, so all derivatives of the density vanish. Eqs.(2.1) and (2.2) are simplified to the Navier-Stokes equations for isothermal, incompressible, Newtonian fluid motion:

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right) = -\nabla P + \eta \nabla^2 \mathbf{u} + \mathbf{f}, \quad (2.7)$$

$$\nabla \cdot \mathbf{u} = 0. \quad (2.8)$$

Eq.(2.7) is usually referred to as the momentum conservation equation and Eq.(2.8) as the mass conservation or continuity equation. The left-hand side of the momentum equation is an acceleration term. The term $(\mathbf{u} \cdot \nabla) \mathbf{u}$ is nonlinear. The existence of nonlinearity requires that the equation is solved numerically for most real situations — analytic solutions exist in certain limits only. Nonlinearity is also the contributor to turbulence. The right-hand side of the momentum equation is the sum of the forces acting on the fluid. It is noteworthy that the viscosity term is represented by the Laplacian of the velocity field, which means that in Newtonian fluids, viscosity is diffusion of momentum.

We have used Finite-Difference approximations applied to both space and time. In particular the marker-and-cell (MAC) mesh (Harlow and Welch 1965)

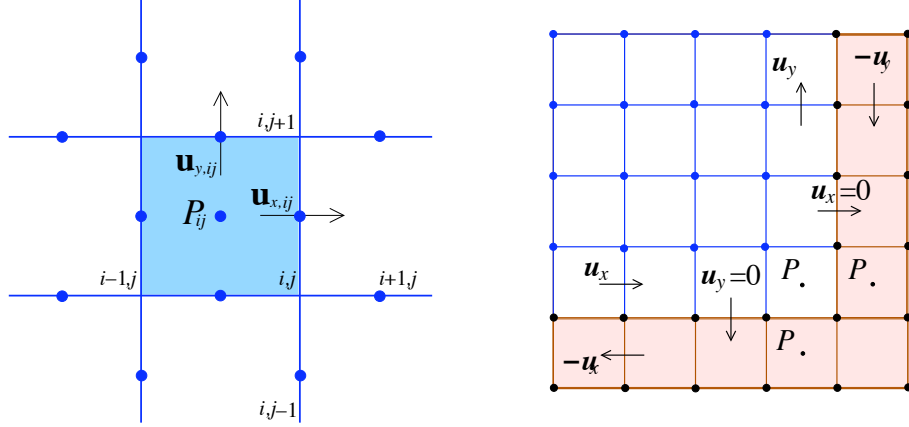


Fig. 2.1: Left: the staggered MAC grid in 2D used for discretising a fluid in space. The pressures are defined at the centre of each cell whereas the fluid velocities are defined at the cell boundaries. Right: part of the fluid grid near two boundary walls. The shaded cells form the no-slip boundary at the walls and the rest are cells occupied by the fluid. Both the pressures and the velocities must vanish at the boundary. The boundary conditions required are illustrated.

was used as the base for the spatial finite-difference discretisation. The time evolution and the actual approximate solution to the Navier-Stokes equations is achieved in two steps using the projection method (Höfler and Schwarzer 2000). We describe each in more detail.

2.2.2 Staggered Marker-And-Cell Grid

The staggered MAC grid (Harlow and Welch 1965) is a regular mesh which divides the region into unit square (2D) or cubic cells (3D). The field variables are the fluid pressure and velocity. Vorticity and streamfunction are not explicitly included in this calculation. The pressures are defined at the centre of each cell whereas the velocities are shifted by half a cell pointing outwards, defined at the cell boundaries, as shown in Figure 2.1 (left). When values are needed at points other than where they are defined (for example the pressure at a cell boundary or the velocity at the centre of a cell) then an interpolation takes place from adjacent cells values.

In most of our simulations we use *no-slip* boundary conditions for the edges of the simulated region in order to model a finite container. The fluid is defined on the staggered MAC grid and an extra layer, one grid-cell thick around it accounts for the sides of the container. If the fluid occupies an area of $N_x \times N_y \times N_z$ grid

cells, in the code a grid of size $(N_x + 2) \times (N_y + 2) \times (N_z + 2)$ is defined. For no-slip boundary conditions the grid cells which make up the boundary and the adjacent fluid ones must have the same pressures so as to avoid pressure gradients driving fluid *into* or *out of* the walls. Similarly, the velocities of the fluid *at* the boundary must vanish. Part of the grid and the boundary conditions are shown in Fig. 2.1 (right). Once the fluid has been spatially defined, the Navier-Stokes equations can be numerically solved in time.

2.2.3 Projection method

The projection method is a finite-difference technique which can be used for solving the Navier-Stokes equations numerically. It was first proposed by Chorin (1968) and Temam (1969) and was further modified for the particle-template model by Höfler and Schwarzer (2000). In the Navier-Stokes equations there are two unknowns, the velocity field $\mathbf{u}$ and the pressure P . The idea behind the projection method is that in the first stage, an intermediate velocity is computed at each time-step ignoring the pressure, and in the second the pressure is used to project the intermediate velocity onto a space of divergence-free velocity field to get the next update of velocity and pressure. Note that the intermediate velocity is not subjected to the continuity constraint of Eq.(2.8).

More specifically, the time derivative of the velocity is split into two components and each is evaluated separately, by employing a fictitious intermediate velocity $\mathbf{u}^*$, which has no physical meaning. The intermediate velocity $\mathbf{u}^*$ is used to split the momentum equation Eq.(2.7) into two, in the following way:

$$\frac{\partial \mathbf{u}}{\partial t} = \left(\frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{dt} \right) = \left(\frac{\mathbf{u}^* - \mathbf{u}^n}{dt} \right) + \left(\frac{\mathbf{u}^{n+1} - \mathbf{u}^*}{dt} \right), \quad (2.9)$$

where n denotes the time step advancement. Hence the momentum equation, Eq.(2.7), can be split into two

$$\frac{\mathbf{u}^* - \mathbf{u}^n}{dt} = -(\mathbf{u} \cdot \nabla) \mathbf{u} + \nu \nabla^2 \mathbf{u} + \frac{1}{\rho} \mathbf{f}, \quad (2.10)$$

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^*}{dt} = -\frac{1}{\rho} \nabla P^{n+1}, \quad (2.11)$$

where $\nu = \eta / \rho$ is the kinematic viscosity of the fluid. Mathematically, Eqs.(2.10) and (2.11) are equivalent to Eq.(2.7). The pressure term is omitted in Eq.(2.10)

so $\mathbf{u}^*$ can be computed. Considering the x -component only as an example, $\mathbf{u}_x^*$ is given by

$$u_x^* = \left[- \left(u_x \frac{\partial u_x}{\partial x} + u_y \frac{\partial u_x}{\partial y} + \frac{\partial u_x}{\partial z} \right) + \nu \nabla^2 u_x \right] dt + u_x^n, \quad (2.12)$$

where

$$u_x \frac{\partial u_x}{\partial x} = u_{x,ijk} \left(\frac{u_{x,i+1jk} - u_{x,i-1jk}}{2dx} \right), \quad (2.13)$$

$$u_y \frac{\partial u_x}{\partial y} = \frac{1}{4} (u_{y,ijk} + u_{y,i+1jk} + u_{y,i+1j-1k} + u_{y,ij-1k}) \left(\frac{u_{x,ij+1k} - u_{x,ij-1k}}{2dy} \right), \quad (2.14)$$

$$u_z \frac{\partial u_x}{\partial z} = \frac{1}{4} (u_{z,ijk} + u_{z,i+1jk} + u_{z,i+1jk-1} + u_{z,ijk-1}) \left(\frac{u_{x,ijk+1} - u_{x,ijk-1}}{2dz} \right), \quad (2.15)$$

and

$$\nabla^2 u_x = \frac{1}{dx^2} (u_{x,i-1jk} + u_{x,i+1jk} + u_{x,ij-1k} + u_{x,i+1jk} + u_{x,ijk-1} + u_{x,ijk+1} - 6u_{x,ijk}). \quad (2.16)$$

By the end of the calculation the vector $\mathbf{u}^*$ is known for all cells in the present time-step.

Let us now consider the pressure equation Eq.(2.11). Solving Eq.(2.11) requires knowledge of the pressure P at a time $n+1$. Taking the divergence of both sides

$$\nabla^2 P^{n+1} = \rho \frac{\nabla \cdot \mathbf{u}^*}{dt}. \quad (2.17)$$

The divergence of the velocity $\mathbf{u}^{n+1}$ vanishes because of continuity, Eq.(2.8). Let us define new variable s equal to the RHS of Eq.(2.17)

$$s = \rho \left[\left(\frac{u_{x,ijk}^* - u_{x,i-1jk}^*}{dt} \right) + \left(\frac{u_{y,ijk}^* - u_{y,ij-1k}^*}{dt} \right) + \left(\frac{u_{z,ijk}^* - u_{z,ijk-1}^*}{dt} \right) \right], \quad (2.18)$$

which can be calculated since $\mathbf{u}^*$ is known. The LHS of Eq.(2.17) in finite-difference form is given by

$$\nabla^2 P_{ijk}^{n+1} = \frac{1}{dx^2} (P_{i-1jk}^{n+1} + P_{i+1jk}^{n+1} + P_{ij-1k}^{n+1} + P_{i+1jk}^{n+1} + P_{ijk-1}^{n+1} + P_{ijk+1}^{n+1} - 6P_{ijk}^{n+1}). \quad (2.19)$$

All the pressure terms correspond to the new time step $n+1$. Solving for P_{ijk}^{n+1}

$$P_{ijk}^{n+1} = \frac{1}{6} (P_{i-1jk}^{n+1} + P_{i+1jk}^{n+1} + P_{ij-1k}^{n+1} + P_{i+1jk}^{n+1} + P_{ijk-1}^{n+1} + P_{ijk+1}^{n+1} - dx^2 \nabla^2 P_{ijk}^{n+1}),$$

$$P_{ijk}^{n+1} = \frac{1}{6} (P_{i-1jk}^{n+1} + P_{i+1jk}^{n+1} + P_{ij-1k}^{n+1} + P_{i+1jk}^{n+1} + P_{ijk-1}^{n+1} + P_{ijk+1}^{n+1} - s dx^2). \quad (2.20)$$

Eq. (2.20) is solved using a lattice relaxation method where the new pressure of each cell P_{ijk}^{n+1} is compared to the present pressure of that cell P_{ijk}^n and they have to be equal within a certain accuracy. Alternatively Fourier methods can be employed to provide a solution to the equation by solving the Fourier transform of Eq.(2.18). Numerically this is achieved by using the FFTW3 subroutine library for C, which solves discrete Fourier transforms in one or more dimensions. After the relaxation or the Fourier transform is complete the new pressures P_{ijk}^{n+1} at the next time-step are known. Having the new pressures, Eq.(2.11) can be solved for $\mathbf{u}^{n+1}$. Considering the x -component only

$$u_x^{n+1} = u_x^* - \frac{dt}{\rho} \left(\frac{\partial P^{n+1}}{\partial x} \right),$$

$$u_{x,ijk}^{(n+1)} = u_{x,ijk}^* - \left(\frac{P_{i+1,jk}^{n+1} - P_{ijk}^{n+1}}{dx} \right) dt, \quad (2.21)$$

where the pressures correspond to time step $n+1$. The new velocities are updated and the current time step is completed.

2.2.4 2D Driven cavity flow

In two-dimensions the fluid model can be tested by considering the flow for a 2D driven cavity. In a square cell, the boundary conditions are such that there are three no-slip walls for the velocities and pressures. On the remaining side, the grid-cells that make up the boundary are given a constant velocity in the direction parallel to the boundary which drives a big vortex and smaller recirculation eddies near the edges. We have used a grid 100×100 , with lattice spacing 10^{-4}m and time-step 10^{-5}s . The side of the square box is 10mm . The viscosity and density of the fluid are those of water, $\nu = 10^{-6}\text{m}^2 \text{ s}^{-1}$ and $\rho_f = 1000\text{kg m}^{-3}$. The imposed velocity on the moving boundary is 0.1 m s^{-1} , so the Reynolds number $\text{Re}=ud/\nu$ is 1000. In 2D the streamfunction ψ can be defined as

$$u_x = \frac{\partial \psi}{\partial y},$$

$$u_y = \frac{\partial \psi}{\partial x}. \quad (2.22)$$

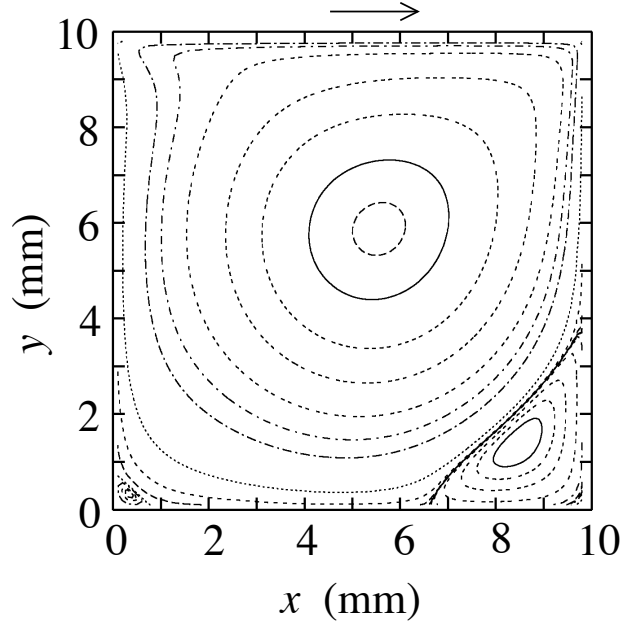


Fig. 2.2: The 2D driven cavity flow for $Re=1000$. The moving boundary is the top one with a velocity 0.1 m s^{-1} .

In Fig. 2.2 we show the contour plot of the streamfunction which is in agreement with known results (Erturk 2005).

2.3 Particle-fluid coupling

The most challenging part of the problem is the way in which the particles interact with the fluid. The fluid-solid coupling comes from the no-slip boundary condition on the surface of the spheres: the fluid at the surface of the sphere is moving with the velocity of the sphere. This is achieved numerically by assuming that the fluid permeates the sphere and that the fluid inside the sphere moves with the instantaneous velocity of the sphere. At a given instant, the force required to keep the fluid inside the sphere moving with the sphere's velocity is calculated from the Navier-Stokes equations Eqs.(2.7) and (2.8). This force is then used to update the solid sphere's position using molecular dynamics techniques, described in Section 2.4. Because the sphere and the fluid have different densities, relative motion between the sphere and fluid is induced.

More specifically, using the projection method for the fluid, once the intermediate fluid velocity $\mathbf{u}^*$ has been calculated the particle template is placed over

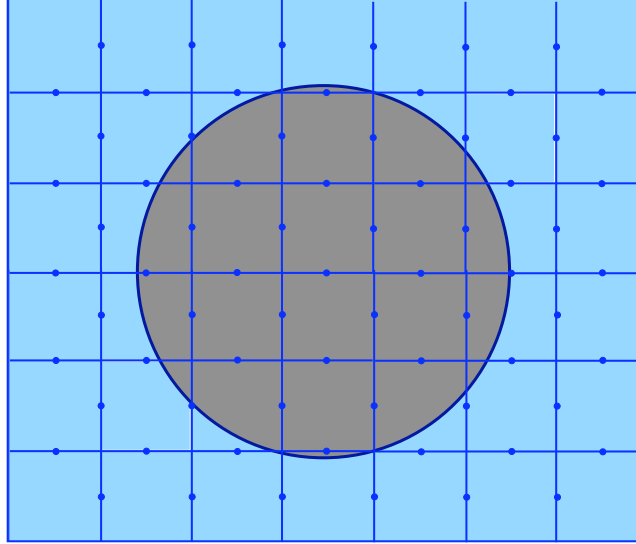


Fig. 2.3: Schematic representation of the particle-template model.

the velocity field. A schematic representation is shown in Fig.2.3. The coupling force between the particle and the fluid is obtained by integrating the stress tensor $\sigma_{ij} = -PI + \mathbb{T}$ over the volume of each particle whilst imposing a no-slip boundary condition on the surface. The force $\mathbf{F}_f$ acting on each particle due to the surrounding fluid is then given by discretising

$$\mathbf{F}_f = \int_V \left(-\frac{1}{\rho} \nabla P + \nu \nabla^2 \mathbf{u} \right) \rho dV. \quad (2.23)$$

$\mathbf{F}_f$ captures both the viscous forces and the buoyancy forces which are experienced by the immersed particle. If the container is vibrated at $\mathbf{a}(t) = A\omega^2 \cos(\omega t)$ then the equation of motion of the particle in the frame of reference of the container is

$$m\ddot{\mathbf{r}} = \mathbf{F}_f + \mathbf{F}_C + m\mathbf{g} - m\mathbf{a}(t). \quad (2.24)$$

$\mathbf{F}_C$ is the cumulative collision force on the particle from any collisions with other solid boundaries or particles. In order to calculate $\mathbf{F}_C$, the collisions are modelled using an elastic repulsive force from overlapping particles in a similar way to molecular dynamics and will be described in Section 2.4.

2.3.1 3D Drag coefficient for falling spheres

The Reynolds numbers associated with the systems we shall investigate in the following chapters, lie in the intermediate range between 2-200. In order to validate

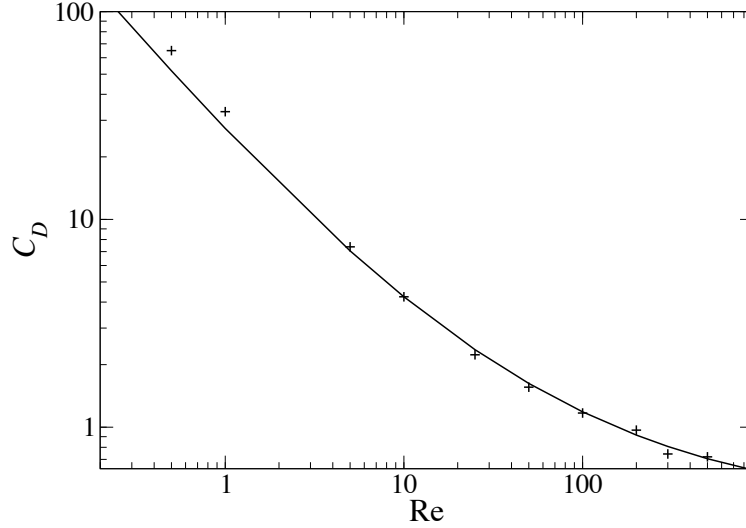


Fig. 2.4: The drag coefficient C_D as a function of the Reynolds number for a sphere moving through water. The solid line is the empirical curve $C_D \approx \frac{24}{\text{Re}} + \frac{6}{1+\sqrt{\text{Re}}} + 0.4$. The points are taken from simulations ran in order to validate the code.

the computational model, we ran simulations for a sphere translating through water at constant velocity v and calculated the drag coefficient C_D which is related to the drag force F_D by

$$C_D = \frac{F_D}{\frac{1}{2}\rho v^2 A} \quad (2.25)$$

where A is the incident area of the object. In Fig. 2.4 we show simulation points for $\text{Re} \in [0.5 - 500]$. The solid line is the empirical curve (White 1991) which is given by

$$C_D \approx \frac{24}{\text{Re}} + \frac{6}{1+\sqrt{\text{Re}}} + 0.4 \quad 0 \leq \text{Re} \leq 2 \times 10^5 \quad (2.26)$$

The current particle-template model has also been validated in the same range of Reynolds numbers in two and three dimensions by Milburn (2006).

2.4 Molecular Dynamics

We shall use Molecular Dynamics methods in order to model the collisions between the spheres and the collisions between the spheres and the boundaries. Molecular Dynamics (MD) is the term used to describe the solution of the classical equations of motion, Newton's laws, for a set of molecules.

In granular systems, Soft Sphere Molecular Dynamics or SSMD is one of the most common methods for describing the evolution and dynamics of the constituent particles, even though they are macroscopic (not molecular) in size.

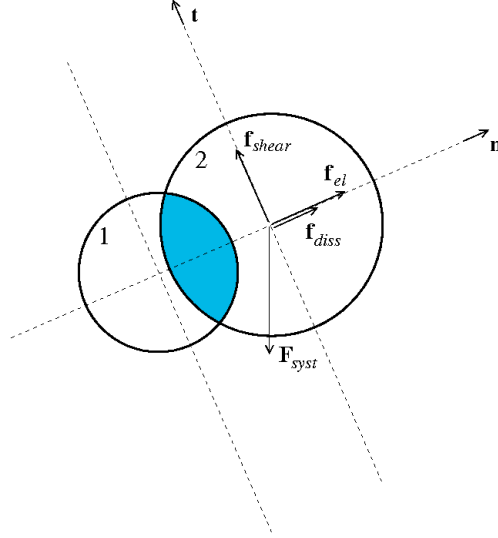


Fig. 2.5: Schematic diagramme of the forces acting during a collision between two particles labelled 1 and 2. The elastic and the dissipative spring forces act in the normal direction $\mathbf{n}$. The shear force acts in the tangential direction $\mathbf{t}$. $\mathbf{F}_{syst}$ is any additional force from the system; the direction here is arbitrary. The shaded area is the overlap between the soft-sphere particles.

The term soft sphere refers to the particles being modelled as such and implies that the particles overlap when they collide and that the impact has a non-zero duration. The interaction potential is short-ranged, repulsive and applies only during collision. As there is a time interval $\Delta t = t - t_0$ during which the collision takes place, the momentum change $\Delta \mathbf{P}$ can be calculated from

$$\Delta \mathbf{P} = \int \mathbf{F}_C(t) dt \quad (2.27)$$

and thus the change in the particles' velocities due to impact can also be calculated. The force $\mathbf{F}_C$ acting on each particle during that time interval must be identified. There are three forces acting on a particle due to collision with another particle and which constitute $\mathbf{F}_C$.

First, there is an elastic repulsive force in the normal direction $\hat{\mathbf{n}}_j$

$$\mathbf{f}_{el} = k_n \delta (\delta / \delta_0)^\nu \hat{\mathbf{n}}_j \quad (2.28)$$

where δ is the penetration depth defined as $\delta = \frac{1}{2}(d_1 + d_2) - (\mathbf{r}_1 - \mathbf{r}_2) \cdot \hat{\mathbf{n}}_j$, d_1 , d_2 , r_1 , r_2 are the diameters and position vectors of particles 1 and 2 respectively, shown in Fig.2.5. k_n is the elastic modulus and δ_0 is a normalisation constant dependent on the non-linearity ν and the dimension.

The second force is a dissipative force in the normal direction, which accounts

for inelastic collisions,

$$\mathbf{f}_{diss} = \gamma_n \dot{\delta} (\delta / \delta_0)^\phi \hat{\mathbf{n}}_j, \quad (2.29)$$

where γ_n is a phenomenological normal viscous dissipation coefficient and $\dot{\delta} = -\mathbf{v}_c \cdot \mathbf{n} = -(\mathbf{v}_1 - \mathbf{v}_2) \cdot \mathbf{n}$ the relative velocity in the normal direction.

The third force is a frictional force acting in the tangential direction $\mathbf{t}$ and the simplest case is equal to

$$\mathbf{f}_{shear} = -\gamma_t \dot{\xi} \mathbf{t} \quad (2.30)$$

where γ_t is the viscous damping coefficient in the tangential direction and $\dot{\xi} = \mathbf{v}_c \cdot \mathbf{t} = |\mathbf{v}_c^{(t)}|$ is the tangential component of the relative velocity, with $\mathbf{t} = \mathbf{v}_c^{(t)} / |\mathbf{v}_c^{(t)}|$. $\mathbf{F}_C$ is the sum of the three components described above, $\mathbf{f}_{el}$, $\mathbf{f}_{dis}$ and $\mathbf{f}_{shear}$.

The total force on each particle is given by

$$\mathbf{F}_{TOTAL} = \mathbf{F}_C + \mathbf{F}_S, \quad (2.31)$$

where $\mathbf{F}_S$ includes any additional forces coming from the system such as gravity or fluid drag. Applying Newton's second law of motion

$$\mathbf{f}_{el} + \mathbf{f}_{diss} + \mathbf{f}_{shear} + \mathbf{F}_S = m\ddot{\mathbf{r}}, \quad (2.32)$$

where m is the mass and $\ddot{\mathbf{r}}$ the acceleration.

The various parameters used in the calculation of the forces ($k_n, \delta_0, \nu, \phi, \gamma_n, \gamma_t$) take different values depending on the system and the numerical way chosen to solve Eq.(2.27). In the next paragraphs we shall discuss the way we have proceeded in order to implement the above model computationally.

2.4.1 Spring-Dashpot Model

In the simplest case, the particles, modelled as soft spheres, collide with a linear spring force which follows Hooke's law so that the parameters are $\nu=1$ and $\phi=0$ and the forces are linear. The repulsive normal force and the dissipative normal force are

$$\mathbf{f}_{el} = k_n \delta, \quad (2.33)$$

$$\mathbf{f}_{diss} = \gamma_n \dot{\delta}. \quad (2.34)$$

Considering only the normal direction, ignoring shear and additional system forces, Eq.(2.32) becomes

$$\begin{aligned} k_n \delta + \gamma_n \dot{\delta} &= -m_{eff} \ddot{\delta} \Leftrightarrow \\ \ddot{\delta} + \frac{\gamma_n}{m_{eff}} \dot{\delta} + \frac{k_n}{m_{eff}} \delta &= 0 \end{aligned} \quad (2.35)$$

which is the differential equation for damped harmonic motion and can be solved analytically for δ . The effective mass term for two particles of masses m_1 and m_2 is

$$m_{eff} = \frac{m_1 m_2}{(m_1 + m_2)}. \quad (2.36)$$

The solution for $\delta > 0$ is

$$\delta(t) = \frac{2v_0}{\omega} \exp\left(-\frac{\gamma_n t}{2m_{eff}}\right) \sin\left(\frac{1}{2} \omega t\right), \quad (2.37)$$

where $\omega = \sqrt{\frac{4k}{m_{eff}} - \left(\frac{\gamma_n}{m_{eff}}\right)^2}$ and $v_0 = \dot{\delta}(0)$. We have assumed that at $t=0$, $\delta=0$. The overlap is positive for as long as the collision lasts so the duration of contact t_c corresponds to $\delta(t_c)=0$ and is equal to

$$t_c = \frac{2\pi}{\omega}, \quad (2.38)$$

which is half the period of the oscillation. Note that here the period $T = 4\pi/\omega$. From the velocity

$$\dot{\delta}(t) = \frac{2v_0}{\omega} \exp\left(-\frac{\gamma_n t}{2m_{eff}}\right) \left[-\frac{\gamma_n}{2m_{eff}} \sin\left(\frac{1}{2} \omega t\right) + \frac{1}{2} \omega \cos\left(\frac{1}{2} \omega t\right)\right] \quad (2.39)$$

we can calculate the coefficient of restitution e_n as the ratio of the change in velocity before and after collision

$$e_n = \frac{\dot{\delta}(t_c)}{\dot{\delta}(0)}, \quad (2.40)$$

which gives

$$e_n = \exp\left(-\frac{\pi \gamma_n}{\omega m_{eff}}\right). \quad (2.41)$$

Using the spring-dashpot model the collision forces can be calculated. In order to solve Eq.(2.32) in time a suitable algorithm is required. Note that by ignoring shear forces in the tangential direction we are not allowing rotational motion of the spheres. As we shall see in later chapters, experimental observations allow for this assumption.

2.4.2 Verlet Algorithm

The usual way to solve differential equations is by advancing the system variables through discrete time steps dt and by approximating the derivatives as finite differences. The Verlet integrator is a direct solution of the second order differential equation of motion Eq.(2.32). It is very popular because it is simple and effective whilst satisfying the desired criteria for MD algorithms. These are: (i) The minimisation of the force calculation, which in MD is by far the most computationally consuming. (ii) Stability, meaning that a small deviation from the correct trajectory will not lead to greater error in subsequent steps. (iii) Time-reversibility is also important because if the simulation is symmetric in time one can trace the particles' trajectories backwards.

The use of time steps dt implies that the quantities under investigation vary smoothly with time so that they can be approximated by their Taylor expansions. Taking $r(t)$ to be the position of the particle at time t and a smooth function of t , we can write down the Taylor series of $r(t)$ about two points $t + dt$ and $t - dt$

$$r(t + dt) = r(t) + \dot{r}(t)dt + \ddot{r}(t)dt^2/2 + \dots \quad (2.42)$$

$$r(t - dt) = r(t) - \dot{r}(t)dt + \ddot{r}(t)dt^2/2 - \dots \quad (2.43)$$

Adding the two equations gives the position of the particle in the next time step

$$r(t + dt) = 2r(t) - r(t - dt) + dt^2\ddot{r}(t). \quad (2.44)$$

It is worth noting that there is no explicit velocity term in Eq.(2.44). The velocity can be calculated from Eq.(2.42) and (2.43), eliminating $\ddot{r}(t)$ and solving for $\dot{r}(t)$

$$\dot{r}(t) = v(t) = \frac{r(t + dt) - r(t - dt)}{2dt}. \quad (2.45)$$

The velocity $v(t)$ can be computed only after the new position $r(t + dt)$ has been determined. It does not directly depend on the present position $r(t)$ but rather on the difference $r(t + dt) - r(t - dt)$ which is what makes the Verlet algorithm time-reversible. For more details on MD simulations we refer the reader to Allen and Tildesley (2000).

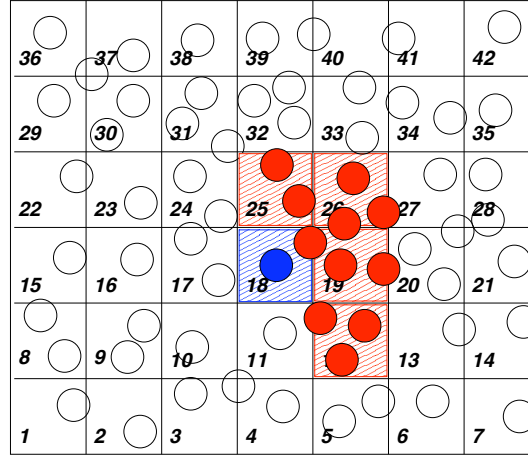


Fig. 2.6: The neighbour list shown for reference particle (blue) in cell 18. Only shaded particles (in red) in the same cell and the four neighbouring cells which are shaded need to be checked for collisions.

2.4.3 Optimisation: Neighbour Link List

The only optimisation technique we have used is the neighbour link list which will be described here. In a compact system where there is a high number of particles in a fairly confined space, it is evident that for instance a particle at one corner of the box will not have managed to collide with a particle at another corner, within one time step, without colliding with a lot of other particles on the way. This simple observation can be used to increase the efficiency of the code, so that the variable calculating the distance between each particle and all the others can compute the distance between each particle and its neighbours only. In order to identify the neighbouring particles, the space of the box is divided into cells where the cell size can be greater or equal to the particle diameter. Both the cells and the particles have an identification index, since they are stored in the code as arrays. The target is to know the positions of the particles in terms of grid cells, i.e. which particles are in each cell. This sorting process is what a link-list method does. We can further increase speed by making full use of Newton's 3rd law and the topology of the grid so that only four neighbouring cells (in 2D), instead of eight, need be checked as shown in Figure 2.6.

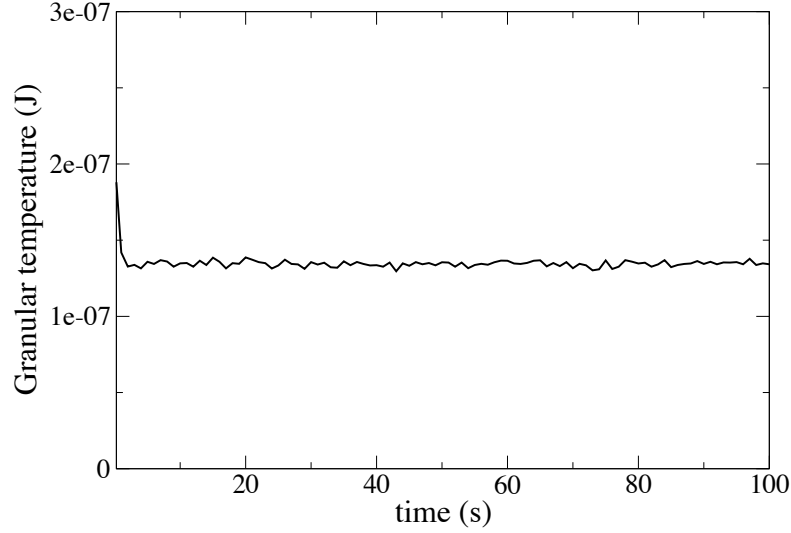


Fig. 2.7: The granular temperature plotted as a function of time for a system of 500 particles. The collisions between the particles are inelastic. A sinusoidally vibrating base provides the energy input.

2.4.4 Validation

As a result of the inelastic collisions, granular systems are highly dissipative and the energy can be described in terms of a granular temperature, defined by Ristow (2000) as

$$T = \frac{1}{N} \sum_{i=1}^N \frac{m_i}{2} ((\mathbf{v}_i - \langle \mathbf{v} \rangle)^2), \quad (2.46)$$

where

$$\langle \mathbf{v} \rangle \equiv \frac{1}{N} \sum_{i=1}^N \mathbf{v}_i. \quad (2.47)$$

The mean velocity is found by averaging over N particles, $\mathbf{v}_i$ and m_i are the velocity and mass of each individual particle respectively. For a further discussion on the granular temperature, definitions that have been formulated and the way it affects various granular systems, see Smith (2001).

The developed MD code was tested to conserve energy when the collisions between the particles were elastic. In order to validate the code in dissipative systems we ran simulations for the motion of 500 identical particles of radius $r = 1\text{mm}$, in a box of size $0.2\text{m} \times 0.2\text{m}$, under the influence of gravity and with a sinusoidally vibrated base at 30Hz . The particles interacted with one another and with the surfaces via a spring force with spring constant $k = 154,020\text{Nm}^{-1}$ and the coefficient of restitution was $e_n = 0.9$. The amplitude of the vibrating

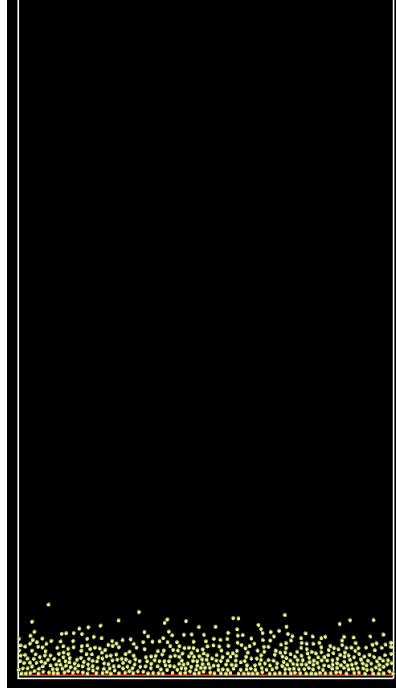


Fig. 2.8: A snapshot of the granular system of 500 particles described in the text. The sinusoidally vibrating base is shown in red. OpenGL interface was used to produce this image.

platform was 1mm and the time step was $\sim 10^{-6}$ s. The granular temperature is conserved as shown in Fig. 2.7 and was also found to agree quantitatively with a Hard Particle Event-Driven code of the same system (Sanders 2006). The code was developed along with the graphics package OpenGL, a snapshot of which is shown in Figure 2.8.

2.5 Discussion

In this chapter we have described the computational model that is used in the rest of the thesis. The aim was to model spherical particles in a fluid-filled container; the spheres being allowed to move and to collide with one another. The fluid and the spheres are modelled using a simplified version of the method developed by Kalthoff *et al.* (1997). The fluid is assumed to be incompressible and described by the 3D Navier-Stokes' equations. These equations are solved numerically using a finite difference approximation and the projection method (Höfler and Schwarzer 2000). The fluid-solid coupling comes from the no-slip boundary condition on the surface of the spheres: the fluid at the surface of the sphere is moving with the velocity of the sphere. This is achieved numerically using the particle-template

model, which does the following. Initially the particle is assumed to occupy a volume of fluid and the force that would act on this volume of fluid due to the surrounding fluid is calculated. That force is then applied to a volume with the density of the particle, which moves with respect to the surrounding fluid. The order in which the program runs is shown in the chart in Fig.2.9.

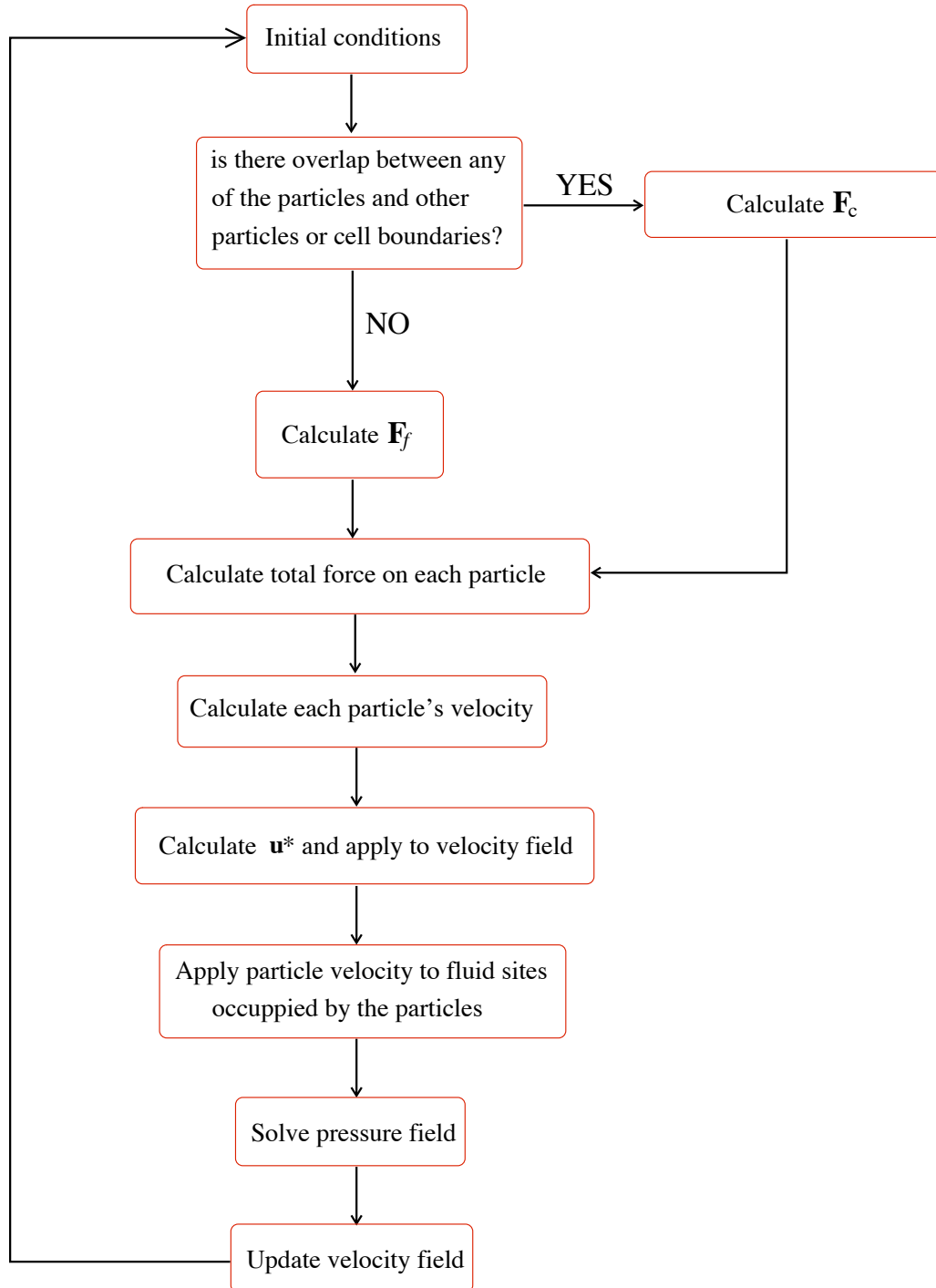


Fig. 2.9: Chart of the algorithm using the projection method to solve the Navier-Stokes equations, a particle-template model for the coupling between particles and fluid and molecular dynamics for the collisions between particles.

Chapter 3

Physics of fluid-particle systems

In this chapter we discuss the physical principles associated with rigid bodies moving in fluids. A brief introduction to relevant studies will be given first. We shall then consider the oscillatory motion of a single sphere at low and high Reynolds (Re) numbers. The nonlinear phenomenon of steady streaming which arises in the intermediate Re range will be explained in detail. The computational model described in the previous chapter will be validated for single-sphere oscillatory systems against published simulations and recent experiments, and some new results will be presented. The interaction of a sphere with solid boundaries, in planes parallel and perpendicular to the axis of oscillation, will be discussed together with results from simulations. The aim of the present chapter is to validate the model specifically in a three-dimensional, oscillatory system. Moreover, the model will be used as a basis for the case of a single oscillating sphere in the geometry and parameter space determined by the experiments, which were in the Reynolds number range 3-120. In subsequent chapters the same model is used to study more complicated environments involving two or more freely-moving, interacting spheres.

3.1 Introduction

In the granular field, controlling the motion of macroscopic particles in the presence of a fluid has been studied since Faraday's time (1830's) because of the numerous potential applications in industry, such as sedimentation (Ramaswamy

2001), transporting and processing of powders, pharmaceuticals and foodstuffs (Wills 1997). Geophysical processes such as the transport of sediment in rivers, volcanic ash flows and sand dunes are also common examples of particle-laden flows.

In many cases fluid-granular systems are forced to flow through pipes, in silos etc. and a large number of grains is usually present. When this is the case, the flow through a granular bed can be described by phenomenological expressions for the flow through porous media. The first to formulate a simple relation between the pressure drop and the flow rate across a porous column was Darcy in 1856 (Darcy 1856). Since then there have been extensions and additions to the model to account for a wider range of applicability such as Forcheimer (1901), Brinkman (1947) and Ergun (1952).

In dilute suspensions where the grains are fewer and the hydrodynamic interaction between each particle and the fluid is important these phenomenological expressions are not sufficient because they describe the granular bed as a whole. A more microscopic description of the particles interacting with the fluid is required, as we shall see in what follows.

The complexity of fluid-particle systems is predominantly related to the motion of the fluid, which is described by the Navier-Stokes equations,

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right) = -\nabla P + \eta \nabla^2 \mathbf{u} + \mathbf{f}, \quad (3.1)$$

$$\nabla \cdot \mathbf{u} = 0. \quad (3.2)$$

The Navier-Stokes equations are nonlinear in u and therefore approximations need to be made depending on the system under investigation. The Reynolds number is the dimensionless parameter which measures the ratio of inertial forces to viscous forces. In the creeping flow limit, at low Reynolds numbers, viscous forces dominate and the Navier-Stokes equations are simplified to the linear Stokes equations by omitting the inertial term.

$$\nabla P = \eta \nabla^2 \mathbf{u} + \mathbf{f}, \quad (3.3)$$

$$\nabla \cdot \mathbf{u} = 0. \quad (3.4)$$

Analytic solutions can then be obtained.

At high Reynolds numbers, if the flow is assumed to be inviscid, the viscous term can be dropped from the Navier-Stokes equations and Euler's equations govern the flow,

$$\rho \left(\frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla \right) \mathbf{u} + \nabla P - \mathbf{f} = 0, \quad (3.5)$$

$$\nabla \cdot \mathbf{u} = 0. \quad (3.6)$$

In steady flows Bernoulli's theorem can be obtained by integrating Euler's equation along a streamline to provide a solution for the pressure distribution. For real fluids at intermediate and high Reynolds numbers both viscosity (even if it is very small) and inertia are equally significant and neither can be neglected. This poses a problem with how to treat the full Navier-Stokes equations, and various numerical techniques have been developed for that purpose, see Chapter 2.

Unsteady flows where the time derivatives of the flow field do not vanish, such as an object accelerating from rest through a fluid or time-periodic flows are more complex and only specific limits can be solved analytically. We are particularly interested in oscillatory flows and we shall focus on them from now on.

A very useful concept in fluid dynamics, first advanced by Prandtl in 1905, is that of the boundary layer. The boundary layer hypothesis states that in the presence of a solid boundary, two regions of flow can be identified: a thin layer close to the boundary called the boundary layer, and a region beyond. Under the hypothesis, the Reynolds number is sufficiently high that viscosity effects are only significant in the boundary layer, which is thin compared to the characteristic size of the boundary, and the rest of the flow is assumed to be inviscid. Batchelor (1967) comments that the boundary layer is in effect the region where the fluid velocity makes a transition from the required value of zero (relative to the solid boundary due to no-slip boundary conditions) to a finite value which is appropriate to an inviscid fluid.

3.2 Oscillatory fluid

A periodic fluctuating fluid flow is often a consequence of an enforced oscillation of a solid boundary or in compressible flows an oscillating sound wave. Let us consider the oscillation of a rigid sphere through a viscous fluid. We assume no-

slip boundary conditions for the surface of the sphere which is oscillating with velocity $U\cos(\omega t)$ in a viscous fluid. The relative motion of the sphere with respect to the fluid produces a flow field. At zero Reynolds number, time-reversibility implies that the flow field which is generated in the first half of the cycle will be cancelled by the flow field generated in the second half of the cycle, therefore producing no net average flow. At moderate Reynolds numbers, however, the fluid is both viscous and inertial and the full Navier-Stokes equations need to be considered. Vorticity is created in the boundary layer, near the surface of the sphere, during every cycle but here the flow fields from opposite parts of the cycle do not cancel. We are dealing with a nonlinear system for which the average fluid velocity field over a cycle is non-zero. As we shall see, in such time-periodic flows it is now well-established that the first-order solution to the velocity is periodic but that there is also a steady part which persists beyond the boundary layer and induces a non-zero flow called steady streaming.

3.3 Streaming flows

The non-zero, time-averaged flow called *steady streaming* may come directly from the action of an oscillatory, non-conservative body force or through the action of Reynolds stresses in the main body of the fluid, produced by no-slip boundaries. In this section we shall give an overview of the studies dealing with such nonlinear time-averaged flows also making the distinction between *acoustic streaming* and *steady streaming*; the former involves acoustic waves and a degree of incompressibility of the fluid and the latter is the non-zero time-averaged flow due to oscillation of no slip boundaries in incompressible fluids.

Nonlinear fluid phenomena of this kind have already been reported by Faraday in 1831. Later, in 1884, Rayleigh gave a theoretical explanation of the streaming produced by standing waves between two plane walls, in a Kundt's tube. The same steady flow pattern was later confirmed experimentally by Andrade (1931a and b), see Fig. 3.1, and Schlichting (1932). These observations formed the basis for a series of experiments, theoretical approaches, and more recently computer simulations on the subject of streaming flows.

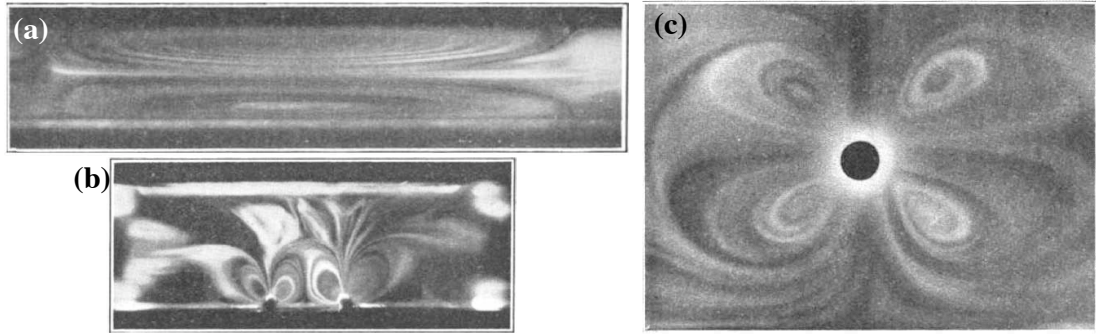


Fig. 3.1: Some of the earliest observations of interesting phenomena in a sounding tube, taken from Andrade (1931a). In (a) the presence of the solid boundary walls is enough to induce steady rotational flows near them. Two spheres act as obstacles to the standing waves in (b) and steady flows are created visualised by smoke particles. In (c) a close up of the steady flow around a sphere in a time-periodic flow observed experimentally for the first time.

There is a number of ways to generate streaming flows in oscillatory systems. The term *acoustic streaming* refers to the steady flow superimposed upon the oscillatory motion by a sound wave propagating in a fluid. A common example is the *quartz wind* which is generated by any source that projects a high-intensity beam of sound into a body of fluid. It was first observed with the use of ultrasonics recently reviewed by Riley (2001). Acoustic streaming in various systems has been studied through experiments (Trinh and Robey 1994) and simulations (Haydock and Yeomans 2001, Rednikov and Riley 2002, Aktas and Farouk 2004). Other examples include the streaming produced by an incident acoustic wave on a cylinder at different Reynolds numbers (Andres and Ingard 1953a and b), or by an oscillatory point source near a sphere (Amin and Riley 1990) as well as the streaming round a spherical drop in an acoustic field (Rednikov *et al.* 2006). Reviews of studies dedicated to acoustic streaming can be found in (Lighthill 1978, Riley 1998, Riley 2001).

In this thesis we are particularly interested in the streaming flow generated when a solid boundary such as an object oscillates in an incompressible fluid, hereafter referred to as *steady streaming*. Cylinders in oscillatory flows have been studied analytically in various limits using boundary-layer approximations, and theoretical approaches such as perturbation theory (Raney *et al.* 1954), successive-approximations methods (Holtsmark *et al.* 1954, Skavlem and Tjøtta 1955), matching solutions (Riley 1965, Stuart 1966), outer-inner expansion tech-

niques (Wang 1968, Bertelsen *et al.* 1973), and matched asymptotic expansions (Amin 1988). They have also been studied numerically using a mesh and finite-difference approximations to solve the full Navier-Stokes equations (Yan *et al.* 1993). The theory has been complemented by various experiments for cylinders in 2D flows (Raney *et al.* 1954, Holtmark *et al.* 1954, Bertelsen *et al.* 1973, Tatsuno 1981).

In three dimensional flows, the motion of an isolated single sphere subjected to an oscillating fluid flow has been studied both analytically and numerically. In particular, methods that have been employed include: boundary-layer approximations and perturbation theory (Lane 1955, Riley 1966), inner-outer expansions (Wang 1965), finite-difference for the time advancement and matched asymptotic expansions for the near and far velocity fields (Mei 1994), spectral methods (Chang and Maxey 1994), a series truncation method (Alassar and Badr 1997), and a spectral element method (Blackburn 2002). Recently, a few experiments, have dealt with 3D flows around an oscillating sphere: by Kotas *et al.* (2007) and by Otto *et al.* (2008). Related experiments have reported the interactions and the patterns formed in oscillatory flows with a large number of particles where steady streaming is expected, and proposed it as a dominant hydrodynamic effect (Voth *et al.* 2002, Wunenburger *et al.* 2002, Thomas and Gollub 2004).

Despite the attention streaming flow has won over the years, it is still not fully understood, involving as it does the nonlinear Navier-Stokes equations, over a large parameter space. We shall define four dimensionless parameters which have been used in the literature: the Reynolds number Re , the inverse Strouhal number ϵ , the streaming Reynolds number Re_s , and M^2 . The radius of the sphere is r , the amplitude of the oscillation is A , the angular frequency is ω and the kinematic viscosity of the fluid is ν . The dimensionless ratios are:

$$\begin{aligned} \text{Re} &= \frac{2A\omega r}{\nu}, \quad \epsilon = \frac{A}{r} \\ \text{Re}_s &= \epsilon \text{Re} = \frac{2A^2\omega}{\nu}, \quad M^2 = \frac{\text{Re}}{\epsilon} = \frac{2r^2\omega}{\nu}, \end{aligned} \quad (3.7)$$

two of which are independent. We shall use Re and ϵ in our experiments and simulations. In Fig. 3.2 we show the parameter space where the analytic, numerical and experimental studies for single sphere systems in oscillatory flows where

steady streaming is generated, have been carried out. (The figure was based on Fig.1 in Otto *et al.* 2008). The upward line with a positive slope is $M^2=1$ and the line with the negative slope is $Re_s=1$.

The solution to the velocity field changes in structure in different limits and thus the form of the steady streaming flow pattern depends on the location of the specific problem in this parameter space. In some cases the structure observed is of the form shown schematically in Fig. 3.3 (a) and depending on the parameters there is a transition to the structure shown in (b). Using perturbation theory, for low amplitudes $\epsilon \ll 1$, Riley (1966) showed that (a) occurs for $M^2 \gg 1$ and $Re_s \ll 1$ and (b) for $M^2 \ll 1$. Rott (1964) in his book on laminar flows suggests that as $|M|^2$ becomes small and vorticity diffuses over a wider region, the innermost region indicated in (a) diffuses over the whole flow field and the streaming is as in Fig. 3.3 (b). Andres and Ingard (1953a and b) have observed a shift from (b) to (a) by increasing the amplitude of the oscillation. Transfer of vorticity associated with the steady streaming takes place mainly by viscous diffusion if Re is small and by convection if Re is large.

Let us consider in detail the streaming flow of Fig. 3.3 (a). The sphere oscillates horizontally in the x -direction as indicated by the dashed line through the sphere and the white double-arrowed line on it. Near the surface of the sphere there are four vortices $\alpha, \alpha', \beta, \beta'$. In three dimensional flows there is rotational symmetry about the axis of oscillation, and so the inner four vortices $\alpha, \alpha', \beta, \beta'$ are actually cross-sections through two vortex rings labelled $\alpha\alpha'$ and $\beta\beta'$. In other words α and α' are cross-sections of a single vortex ring $\alpha\alpha'$. These two vortex rings result from the no-slip boundary condition between the surface of the sphere and the fluid, which are moving relative to each other. We shall call this non-zero average flow *inner streaming*, sometimes also called *primary streaming*. The initially undisturbed fluid further out will start to circulate as well, as a result of the inner streaming. The vortex ring labelled $\alpha\alpha'$ will generate the outer vortex ring AA' . Similarly $\beta\beta'$ will produce BB' . The outer vortex rings circulate in the opposite direction and are spatially much bigger. This we shall call *outer streaming* or *secondary streaming*. A schematic diagram showing the three-dimensional orientation of the outer streaming flow is shown in Fig. 3.4.

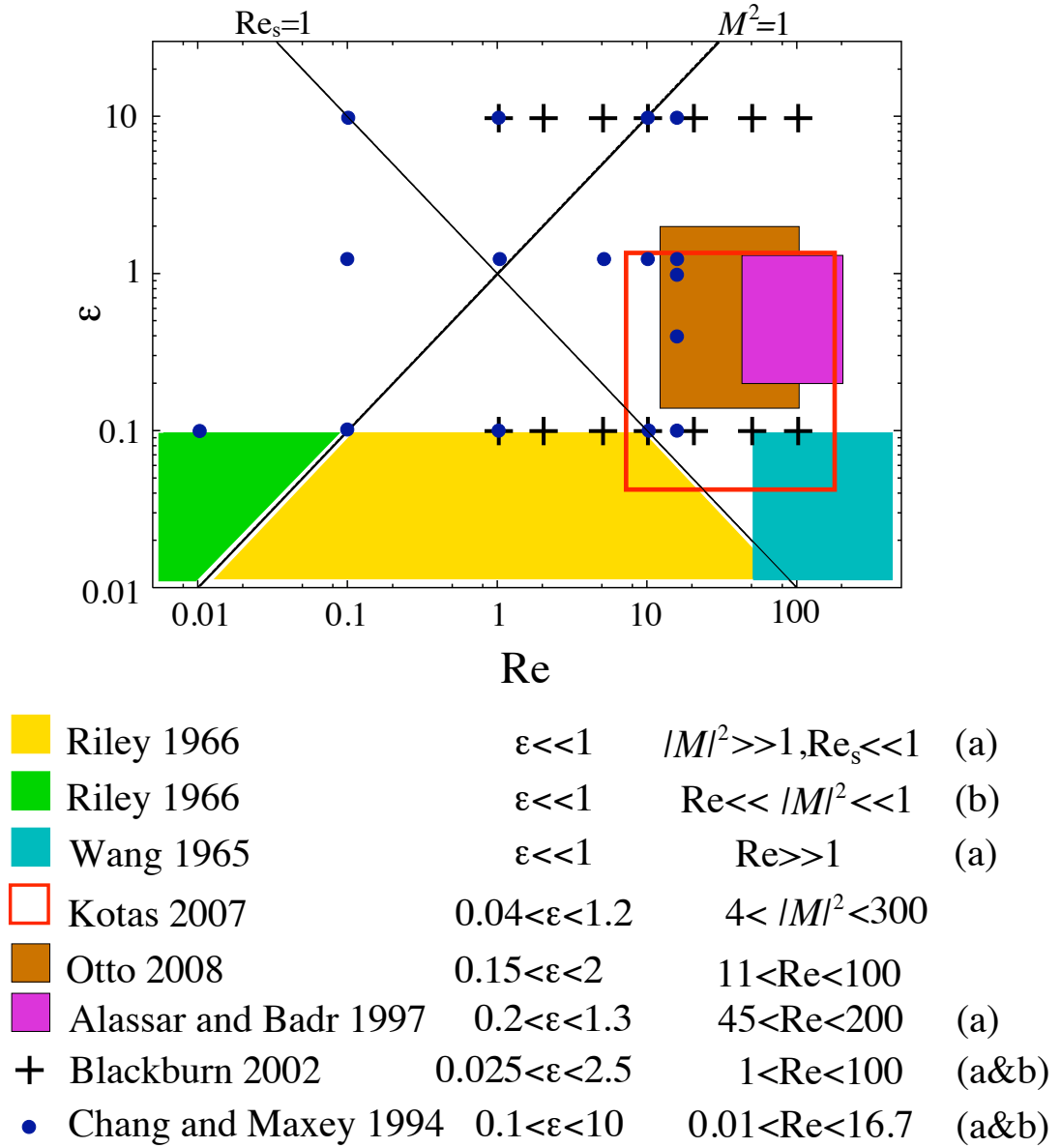


Fig. 3.2: Parameter space showing the regions where various studies have been conducted for a single sphere oscillating in a fluid.

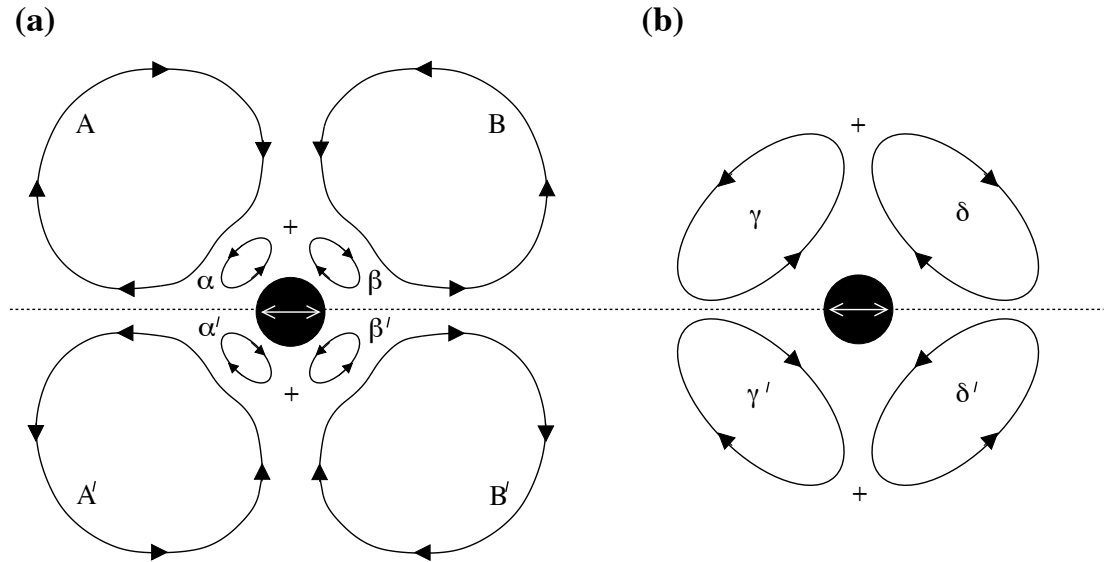


Fig. 3.3: A schematic diagram showing the streaming flow for a single oscillating sphere in the plane through the sphere. Two types of streaming flow exist shown in (a) and (b) which depends on the region of the parameter space. Crosses indicate stagnation points.

As the amplitude and the Reynolds number get smaller, the streaming shown in (a) will shift towards (b), the inner streaming expanding spatially and the outer streaming getting weaker. In the limit shown in Fig. 3.3 (b) only the inner streaming is present, as the outer streaming is too weak. The structure shown in (a) is more general for the systems we will be looking at.

3.4 Simulating oscillatory fluid particle motion

In this section we are going to show results from our simulations for the oscillatory motion of a single sphere in a fluid, using the computational model described in Chapter 2. First we present vector plots of the steady streaming flows comparing our results with experimental data. We then measure the drag coefficient for an oscillating sphere and compare with known values in the literature.

3.4.1 Steady streaming flows

There are very few experimental studies for three-dimensional steady streaming flows. We shall discuss the results of Kotas *et al.* (2007) and Otto *et al.* (2008) because they are recent and because both study the flow around a single oscillating sphere at finite Reynolds numbers and amplitudes, and provide visualisation and

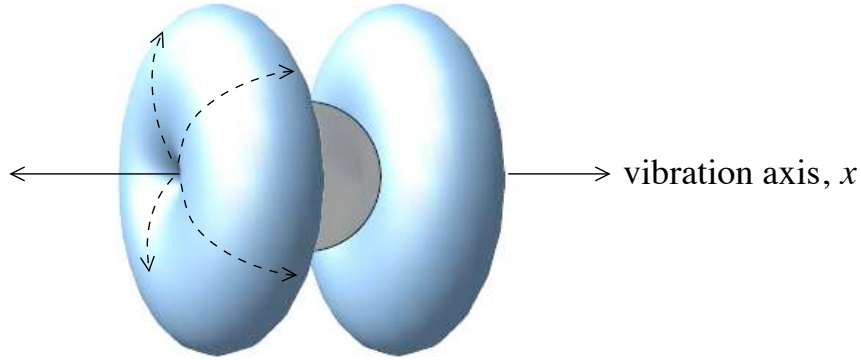


Fig. 3.4: Schematic diagram showing the three-dimensional nature of the flow. For simplicity we show only the outer streaming flow. The sphere is oscillating along the vibration axis as indicated, generating a torus of fluid on either side. Taking a slice through the centre of the sphere in x - y plane would give the outer flow shown in Fig. 3.3 (a). Note that the inner streaming flow (not shown) also consists of two vortex rings which are smaller in size and swirl in the opposite direction to the outer ones shown here.

velocity data for the flow fields.

Kotas *et al.* (2007) conducted experiments in which various spheroids were vertically oscillated in a fluid-filled container. We are only interested in the experiments for spheres so our discussion is limited to those. The sphere was glued onto a metal rod which was then mounted on a shaker. The vibratory conditions were varied and each time the average flow field was recorded and visualised. Their aim was to extract the three-dimensional streaming flows and measure the extent of the inner region, the inner steady streaming. We shall try to simulate their system but let us see first the details of their experiment.

The tank filled with fluid was $25 \times 50 \times 30$ cm, the sphere radius was 1.27 cm and the oscillation was in the vertical, z -direction. Gravity did not influence the motion of the sphere. The parameters given in Kotas *et al.* (2007) were: $\nu = 1.69 \times 10^{-4} \text{ m}^2 \text{ s}^{-1}$, $\epsilon = 0.1$, $M^2 = 168$ and $\text{Re} = 16.8$, and frequency range 2-15 Hz. Note that the system we have simulated is identical to the experimental set-up of Kotas *et al.* (2007) with the exception of the vibrating rod on which the sphere was attached in the experiments. The average steady streaming flows from our simulations are shown in Fig. 3.5 (a); the results taken from Kotas *et al.* (2007)

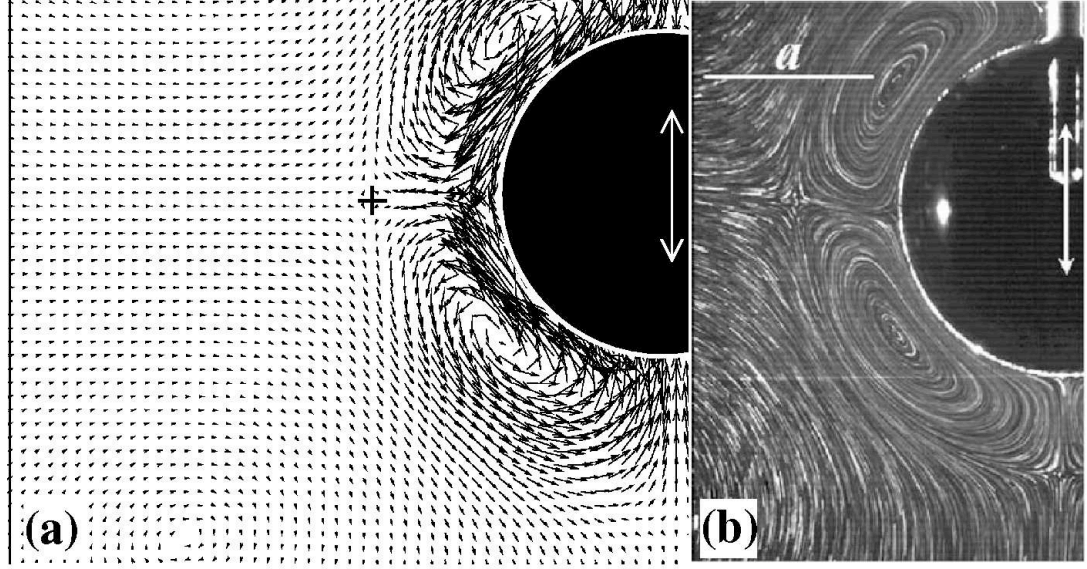


Fig. 3.5: Qualitative agreement of the steady streaming flow between (a) present simulations, (b) experiments by Kotas *et al.* (2007) for a sphere radius $r=1.27\text{cm}$ oscillating in a finite container filled with fluid. $\text{Re}=16.8$, $M^2=168$ and $\epsilon=0.1$. The stagnation point distance from the surface of the sphere is (a) $T=0.77r$, (b) $T=0.6r$.

are shown in Fig. 3.5 (b). In both simulations and the experiment we can see the non-zero average flow in the region near the sphere. In our simulations the outer steady streaming flow can also be seen swirling in the opposite direction to the inner streaming flow. Our results are in qualitative agreement with those shown in (b) and can also be compared to the predicted structure in Fig. 3.16 (a). We also compare the streaming flows from our simulations with the results of Kotas *et al.* for a different set of parameters: $\epsilon = 0.2$, $M^2=80$ and $\text{Re}=16.8$; see Fig. 3.6 (a) and (b).

The extent of the inner region of the flow (the inner streaming) is characterised by the distance from the surface of the sphere to the stagnation points beyond which the flow has the opposite direction (the outer streaming). The radial stagnation point distance which is perpendicular to the axis of oscillation is usually considered. In the experiments of Kotas *et al.* (2007) it is the only one because the flow in the direction of the oscillation axis is distorted by the rod. Kotas *et al.* (2007) measured the average flows and the stagnation point distance, T , for various vibratory conditions and different spheroids. Using our earlier definitions for the dimensionless parameters, their results collapse according to the scaling $T=Cr/M^2=C\nu/2r\omega$, $C=92$. In other words there is no dependence on the

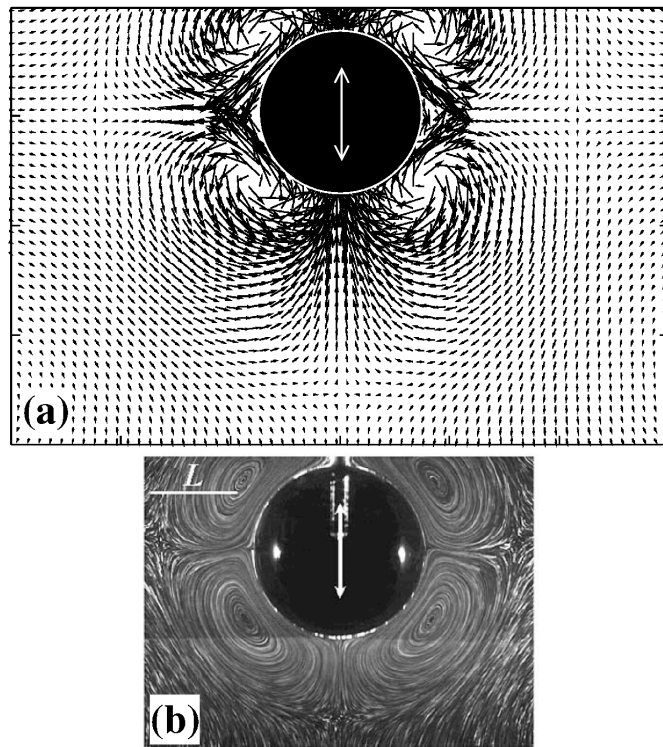


Fig. 3.6: Comparison of the steady streaming flow between (a) present simulations and experiments by Kotas *et al.* (2007) for a sphere radius $r=1.27\text{cm}$ oscillating in a finite container filled with fluid. $\text{Re}=16.8$, $M^2=80$ and $\epsilon=0.2$. For clarity the velocity vectors in (a) have been scaled by the square of the distance to the centre of the sphere.

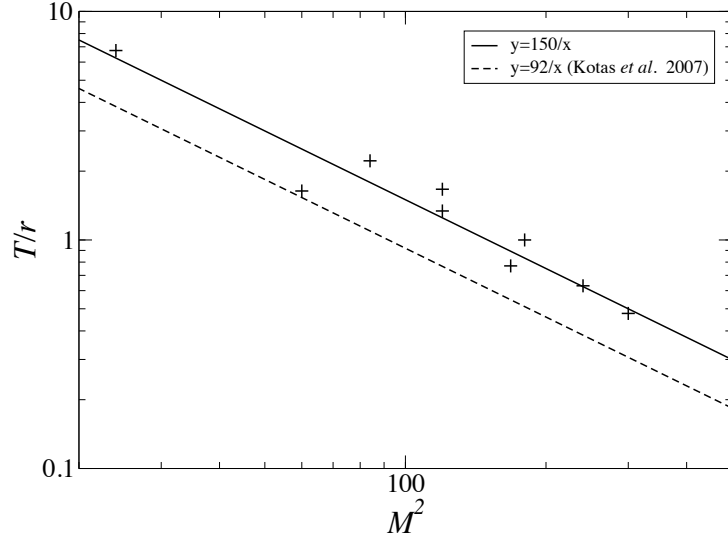


Fig. 3.7: Logarithmic plot of the extent of the inner region, the distance from the surface of the sphere to the radial stagnation point T , as a function of M^2 . The plus signs are taken from our simulations. The dashed line shows the experimental collapse reported by Kotas *et al.* (2007).

amplitude of oscillation and the only important parameter seems to be the ratio ν/ω , which is the square of the boundary layer thickness, $\delta = \sqrt{\nu/\omega}$. We have run simulations for the same range of vibratory conditions, for spheres of diameter 2.54 cm. After measuring the average fluid flows we have also calculated the stagnation point distances T . In Fig. 3.7 we show our simulation results (solid line) on a logarithmic scale, together with the results from Kotas *et al.* (2007) (dashed line). We find that our data also scale in the same way $T = Cr/M^2$, but our constant is higher $C = 150 \pm 1$. Kotas *et al.* commented that simulations usually tend to overestimate the stagnation point distance because of transient effects: usually only a few oscillation cycles are simulated compared to experiments. They also mention a private communication which indicated that the inner region after 10 oscillations is about 10% larger than after 100 oscillations. In our simulations we let our spheres oscillate for about 50 cycles. Our overestimate of the stagnation point distance may be related to the fact that we cannot let the simulation run for over 100 cycles.

More recently, Otto *et al.* (2008) conducted a series of experiments measuring the steady streaming flows around one and two spheres using three-dimensional particle tracking velocimetry, with a similar arrangement to Kotas *et al.* (2007). They studied how the flow field changes when a boundary is brought near the

oscillating sphere. Their goal was to get a better understanding of the experiments by Voth *et al.* (2002) on self-organisation, in which the particles bounced off the bottom surface of a fluid-filled container forming various structures (Voth *et al.* 2002).

Otto *et al.* (2008) observed the flows around a sphere far from boundaries, a sphere which was oscillating vertically (in the z -direction) in a container filled with fluid. The container size was $30 \times 30 \times 20$ cm and the sphere radius, $r=0.955$ cm. The time-averaged fluid flows for $Re=16.7$, $M^2=24$, $Re_s=46.8$ and $\epsilon=1.4$ are shown in Fig. 3.8 (a). Our simulation results of the vector fluid flow for the same system are shown in Fig. 3.8 (b). Qualitative agreement is evident: there is an inner and outer region swirling the right way. The crosses in (a) and (b) indicates the stagnation point. The stagnation point distance T has also been plotted against radial distance from the surface of the sphere, Fig. 3.9. Here, positive indicates flow away from the sphere due to the inner streaming, and negative indicates flow towards the sphere due to outer streaming.

Alassar and Badr (1997) performed simulations for an oscillating sphere studying the fluid field and streaming flows for a range of Re and ϵ . They discuss under what conditions the streaming consists predominantly of the inner region Fig. 3.16 (b) or both inner and outer (b). For $Re=50$ and $\epsilon=1.274$ we have plotted the average streaming flow from our simulations in Fig. 3.10 (a) and the streamfunction taken from Alassar and Badr (1997) in (b). In our computational model we do not have an explicit term for the vorticity or the streamfunction so it is more accurate to look at the average velocity fields.

3.4.2 Drag coefficient

For a single sphere oscillating in a fluid the drag coefficient is given by

$$C_D = \frac{F_D}{\rho U_0 \pi^2}, \quad (3.8)$$

where F_D is the drag force, ρ is the fluid density and U_0 is the amplitude of the free-stream velocity, $U_0 = A\omega$, A is the amplitude and ω the angular frequency. The drag coefficient is composed by two parts one due to pressure and one due to viscosity. In order to validate our computational model (see Chapter 2 for

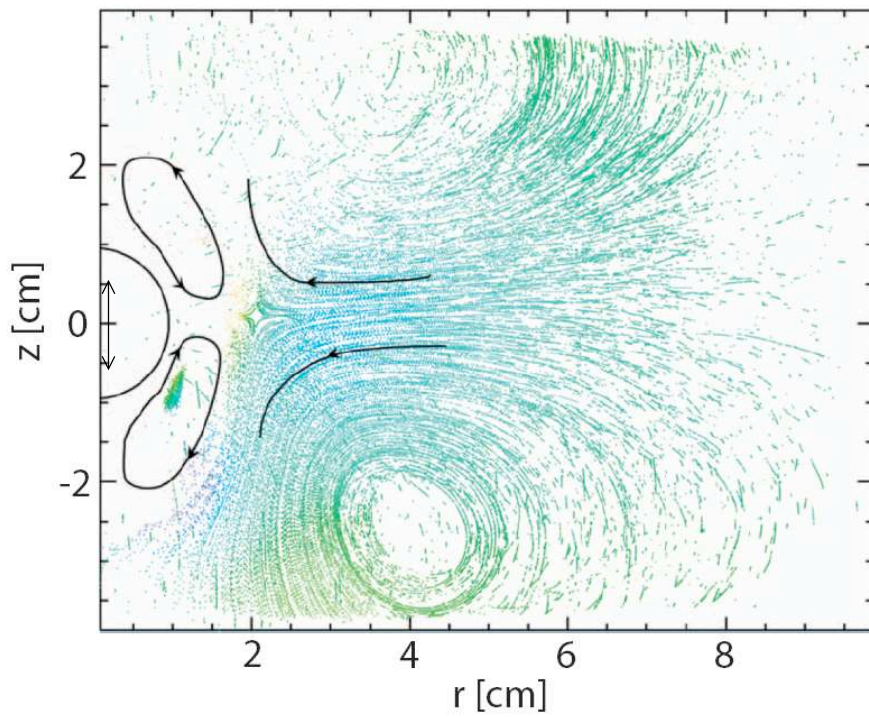
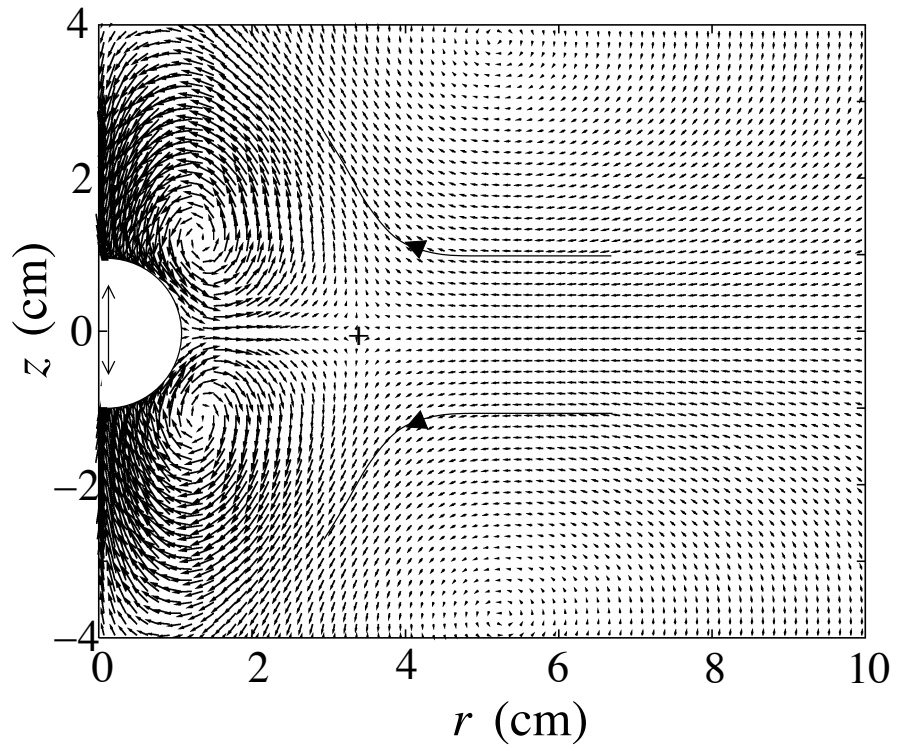


Fig. 3.8: Time-averaged streaming flow for a sphere oscillating vertically in a fluid-filled tank, at $Re=16.7$ and $\epsilon=1.4$.

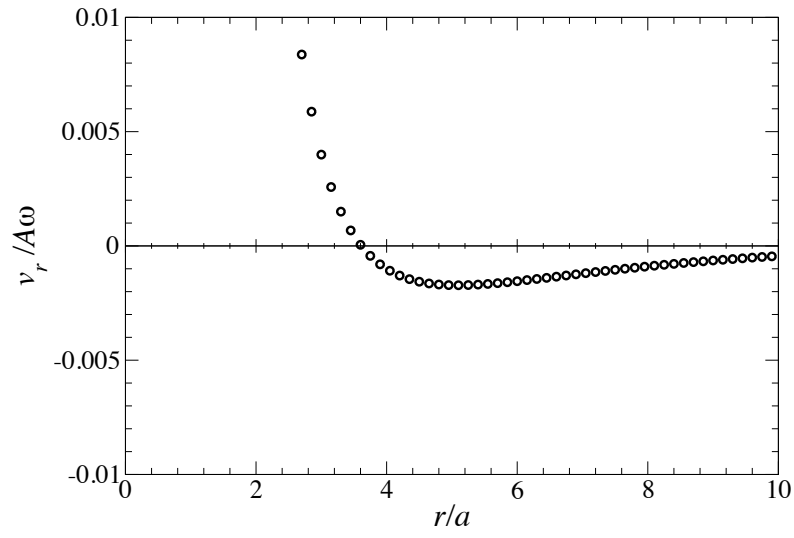


Fig. 3.9: Steady inflow velocity v_r versus r along the axis perpendicular to the vibration. $\text{Re}=30$, $\epsilon=1.4$, $\text{Re}_s=42$, $|M|^2=24$.

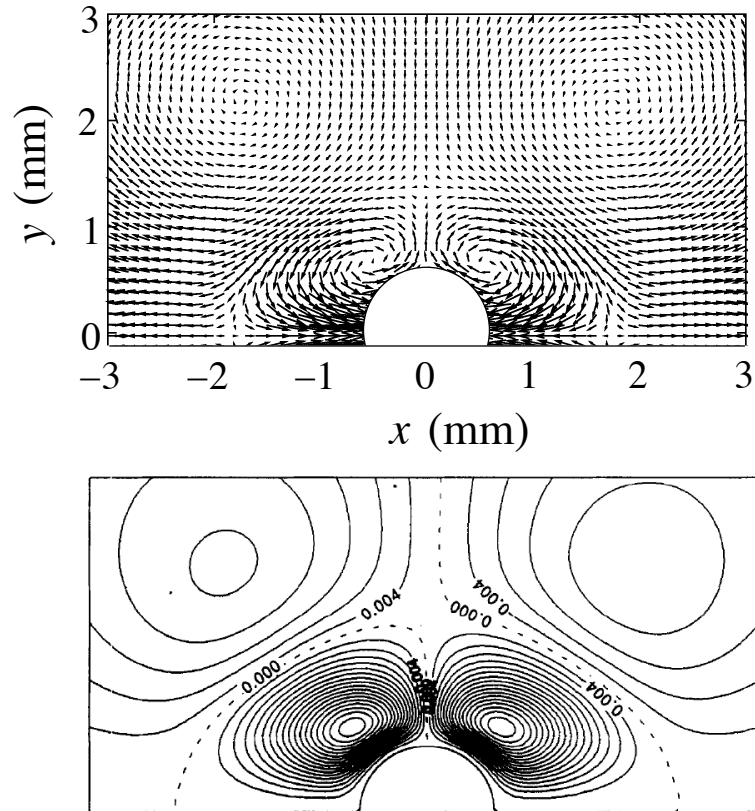


Fig. 3.10: The average fluid flow computed using our simulations in (a) and the streamfunction from Alassar and Badr (1997) in (b) for an oscillating sphere at $\text{Re}=50$ and $\epsilon=1.274$.

details) we have compared our simulation results with the numerical results of Alassar and Badr (1997) and Chang and Maxey (1994). In these two studies (which are in agreement with each other) the drag force and fluid field for an oscillating sphere was solved using a series truncation method (Alassar and Badr 1997) and spectral methods (Chang and Maxey 1994) in an infinite fluid.

Let us consider a sphere of radius $r=0.5\text{mm}$ oscillating in a fluid initially at rest in a finite box of side $X=10\text{mm}$. The lattice spacing and time-step in the simulation are taken to be $Dx = 1.0 \times 10^{-4}\text{m}$ and $Dt = 1.0 \times 10^{-5}\text{s}$ respectively. The sphere oscillates and the fluid flows are generated by the relative motion of the sphere with respect to the fluid. The drag force is the force which acts on the sphere opposing its motion through the fluid in the direction of oscillation. In the simulation this force is calculated every time-step by integrating the stress tensor around the sphere, see Eq.(5.2). The dimensionless drag coefficient given by Eq.(3.8) is plotted in Fig. 3.11 as the solid line; the curve from (Alassar and Badr 1997, Chang and Maxey 1994) is also shown for reference (dashed line). In both cases the vibratory conditions and viscosity correspond to a Reynolds number ($=A\omega d/\nu$) $\text{Re}=16.7$ and $\epsilon=1.6$. In Fig. 3.12 we show a close-up of the pressure C_{DP} and viscous C_{DV} components for the same curve, over one cycle of oscillation. The free-stream velocity, v_f , which in the case of an oscillating sphere is the velocity of the sphere, is also plotted as a dashed line. Although our estimate for the drag coefficient is out by 17% compared to the Alassar and Badr (1997) value (both shown in Fig. 3.11) it is evident that there is fairly good qualitative agreement. We would like to note that the present simulation method (the particle-template model) is used for the first time in oscillatory viscous flows where steady streaming is generated. In Fig. 3.12 we see a phase lead of the pressure and viscous components to the drag, over the free-stream velocity. The phase lead is in agreement with both Chang and Maxey (1994) and Alassar and Badr (1997). The viscous force changes sign before the free-stream velocity and that is attributed by Chang and Maxey (1994) to the recirculation region formed following separation during the decelerating period of the cycle. The drag coefficient, with its pressure and viscous components and the free-stream velocity are plotted in Fig. 3.13 for $\text{Re}=50$ and $\epsilon=1.274$.

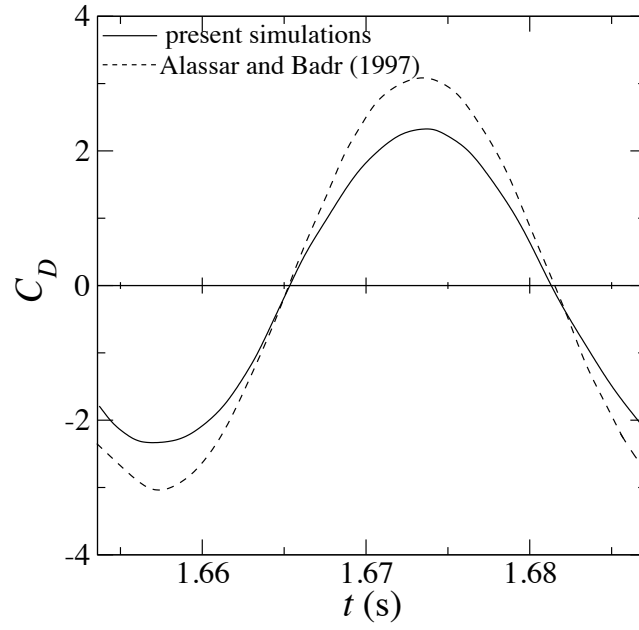


Fig. 3.11: The drag coefficient over one oscillation cycle for $Re=16.7$ and $\epsilon=1.6$ after 50 cycles. The solid line is from our simulations and the dashed line is the drag coefficient given by Alassar and Badr (1997) and Chang and Maxey (1994). Our data has been smoothed to reduce noise.

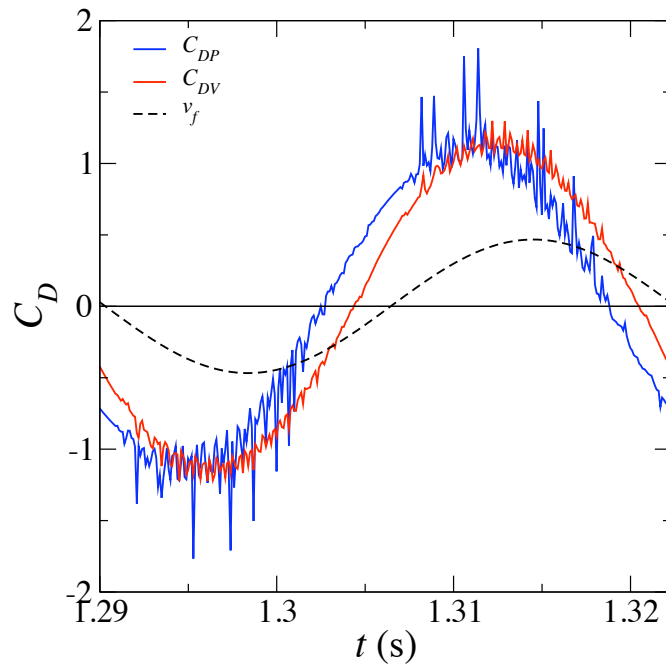


Fig. 3.12: The pressure C_{DP} and viscous C_{DV} components of the drag coefficient over one cycle of oscillation for $Re=16.7$ and $\epsilon=1.6$ after 50 cycles. The freestream velocity is also plotted in the dashed line; for clarity it has been scaled up.

Chapter 3

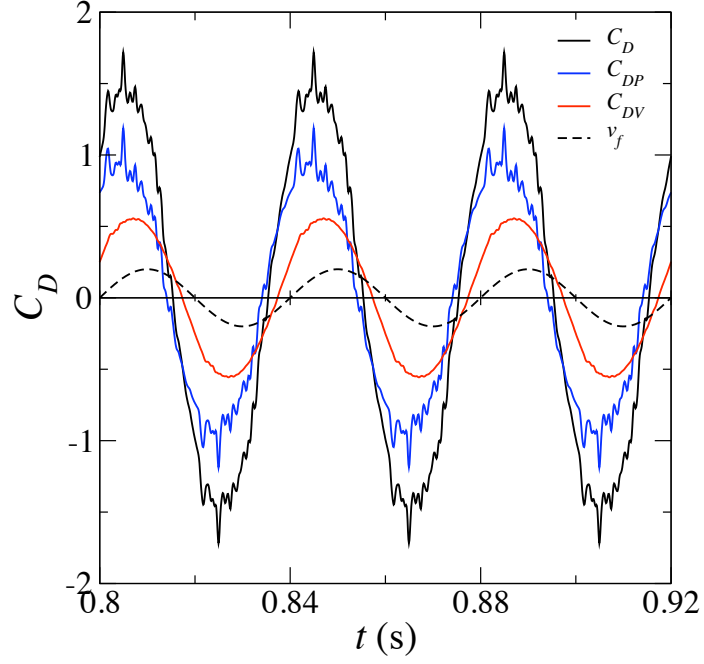


Fig. 3.13: The drag coefficient and its components pressure and viscous for $Re=50$ and $\epsilon=1.274$.

In order to try to pinpoint where the discrepancy comes from we have run a number of simulations changing one parameter at a time. We keep $Re=16.7$ and $\epsilon=1.6$ fixed. In Fig. 3.14 we show the drag coefficient for (a) $Dx = 1.0 \times 10^{-4}s$, $Dt = 1.0 \times 10^{-5}s$ and $X=10mm$. (It is the same curve as in Fig. 3.11). Keeping everything else fixed we have varied the lattice spacing (b) $Dx = 2.0 \times 10^{-4}m$ and (c) $Dx = 0.5 \times 10^{-4}m$; the time step (d) $Dt = 2.0 \times 10^{-5}s$ and (e) $Dt = 0.5 \times 10^{-5}s$ and the box side (f) $X=20mm$ and (g) $X=5mm$. We can see that only the grid spacing has a significant effect on the drag force. In fact it seems that the better the resolution is, the closer the drag coefficient curve is shifted towards the predicted value shown in dashed in Fig. 3.11. The noise also almost completely goes away when the lattice spacing is reduced as can be seen in (c). However, the difference between (a) and (c) is very small and (c) is extremely computationally intensive. The resolution corresponding to (a) $Dx = 1.0 \times 10^{-4}s$ is ~ 13 grid points per sphere diameter. In the rest of the thesis, we will keep the resolution very close to this value. In other words, we shall vary the sphere radius and the box size, keeping the resolution between 10-14 grid points per sphere diameter. The time step will be fixed at $Dt = 1.0 \times 10^{-5}s$.

It is evident that our simulation method is not perfect. Our estimates for

the drag coefficient and its components are consistently smaller than the values given by Alassar and Badr (1997), and Chang and Maxey (1994). However we remind the reader that our simulations are done in a finite box whereas in both the aforementioned studies the fluid is assumed to be infinite. Moreover our task is not to develop a complicated model to predict an accurate value for the drag coefficient. Rather, our aim is to develop a simple and accurate enough model which will do the following: capture the behaviour of the system; allow more than one sphere to move freely in an oscillating box, so that it can interact and collide with other spheres and the walls of the container. Such a model allows us to investigate the physical mechanisms of such a system. The rigorous methods which provide extremely detailed descriptions of the flow fields and give accurate estimates for the drag coefficients are not able to carry out such a program. We, therefore, trust that the discrepancy in the quantitative value of the drag is not of great importance considering what we are aiming to do in the remainder of the theses.

3.5 Oscillations Near Boundaries

Otto *et al.*'s (2008) experiments ultimately studied the flow field around a vertically-oscillating sphere when a flat surface acting as a solid boundary was placed close to the sphere. This flat surface was at right angles to the axis of oscillation and was brought near to the sphere to the point where the bottom surface and the sphere are almost just touching so that the sinusoidal oscillation was not affected. They found that the flow field changes so that in the end the lower part of the streaming flow was no longer present and the inner streaming region on the other side of the boundary extended further from the sphere compared to when the boundary is far away.

In this section, we will describe the geometry of the system we are going to study in the rest of the thesis, shown schematically in Fig. 3.15 and discuss the influence of the boundaries of the container on the oscillating sphere. Note that it is different to the geometries we have discussed so far.

When the sphere is placed in the container it sinks to the bottom due to gravity

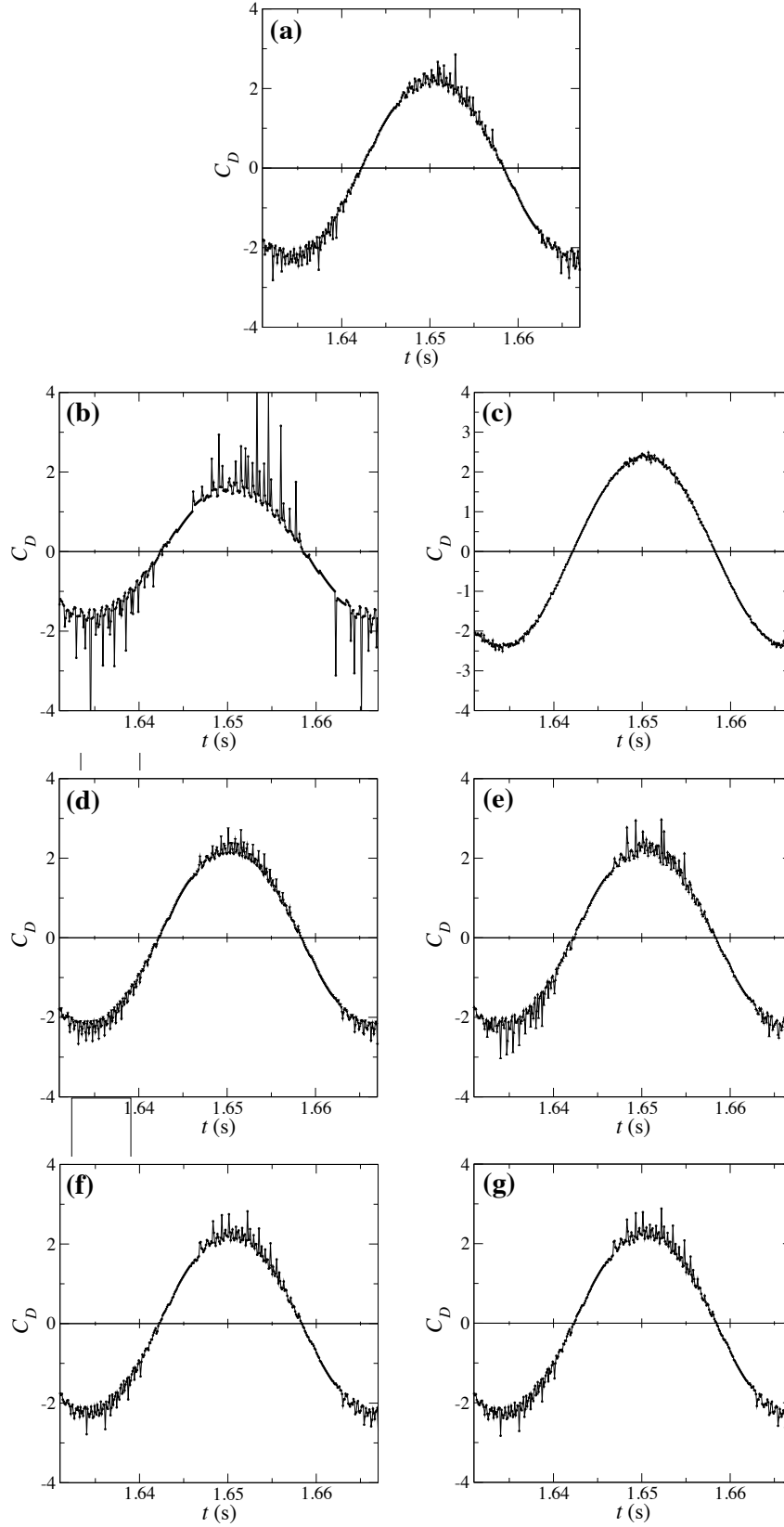


Fig. 3.14: The drag coefficient over one oscillation cycle for $Re=16.7$ and $A/r=1.6$. The parameters are: $Dx = 1.0 \times 10^{-4}s$, $Dt = 1.0 \times 10^{-5}s$ and $X=10mm$. Keeping all else fixed, we vary: the lattice spacing (b) $Dx = 2.0 \times 10^{-4}m$ and (c) $Dx = 0.5 \times 10^{-4}m$; the time step (d) $Dt = 2.0 \times 10^{-5}s$ and (e) $Dt = 0.5 \times 10^{-5}s$; the box side (f) $X=20mm$ and (g) $X=5mm$.

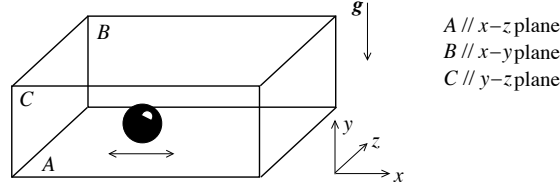


Fig. 3.15: The three plane boundaries A, B, C near the sphere in our geometry. The oscillation is indicated by the double arrowed line. We have drawn the direction of the acceleration of gravity vector $\mathbf{g}$ and x, y and z .

and then slips on the bottom flat surface when horizontal vibration is applied. The planes we shall consider are labelled A, B and C . The sphere is close to the bottom flat surface, A , which is parallel to the oscillation. We study how surface A affects the flow field. Then we shall look at the interactions between a sphere and wall B which is also parallel to the oscillation but there is no gravity in that direction so the sphere is not bound to the wall. Wall C plays no important role, the sphere is just found to bounce off it occasionally.

3.5.1 Bottom surface

In our simulations the spheres are free to move but are prevented from reaching the outer cells of the fluid grid, in the bottom plane, by a contact force which restrains them so that the sphere's surface is at least one lattice spacing from the true cell boundary. In this way we aim to reproduce the geometry of the experiment whilst keeping the computational model simple so that the dominant physical mechanisms can be identified. Lubrication forces or friction could be included but they are known to be complex (Wunenburger *et al.* 2002). There will be more on this topic in the next chapter, but for now we will assume that the spheres are not directly interacting with the bottom plane; they are forced to oscillate very close to it, $Dx \simeq 0.15r$, and in a direction parallel to it, in the x -direction.

We have run simulations for typical values in the parameter space which we are concerned with in the following chapters. Specifically the sphere is 0.5mm radius, the lattice spacing is 7.5×10^{-5} m and the container dimensions are $21 \times 21 \times 3$ mm. The sphere is oscillated in a fluid initially at rest, and the fluid velocity fields are recorded every time-step and time-averaged over one cycle, after 50 cycles to

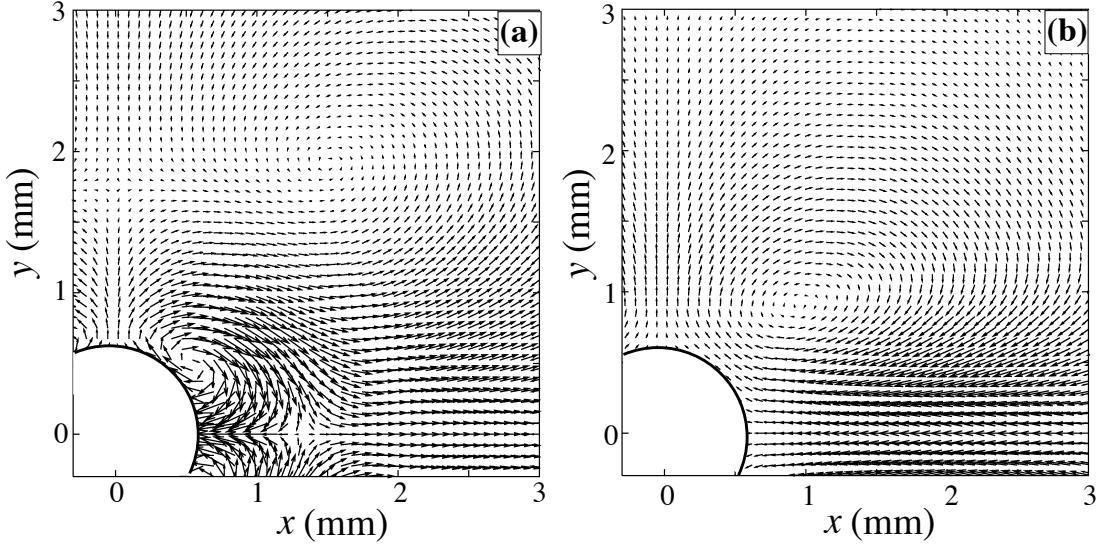


Fig. 3.16: Vector plot of the fluid flow for an oscillating sphere in a plane through the centre of the sphere. The axis of oscillation is the x -axis and the plane of the flow shown is the x - y plane. In (a) $\text{Re}=M^2=78.5$, $\epsilon=1.0$ and in (b) $\text{Re}=25.4$, $M^2=6.7$, $\epsilon=3.8$.

minimise transient effects and make sure that a steady state has been reached. By steady state we mean that the fluid velocities oscillate periodically at the driving frequency. In Fig. 3.16 we show two vector plots of the streaming flows in the x - y plane for (a) $\nu=2.0 \times 10^{-6} \text{m}^2 \text{s}^{-1}$, $f=50 \text{Hz}$, $A=0.5 \text{mm}$, $\epsilon=1.0$ and (b) $\nu=9.4 \times 10^{-6} \text{m}^2 \text{s}^{-1}$, $f=20 \text{Hz}$, $A=1.9 \text{mm}$, $\epsilon=3.8$. The time-averaged streaming flows can be clearly seen and compared to the predicted schematic diagrams shown in Fig. 3.3 (a) and (b). The vector plot shown is in the x - y plane through the centre of the sphere at $z=0.6 \text{mm}$ from the bottom. For clarity, here we only show a quadrant of the flow field and the local velocity vectors are scaled by the distance from the centre of the sphere. It should be noted that the instantaneous fluid flow has only one inner vortex loop which oscillates backwards and forwards around the sphere. This is true for both sets of parameters; in the case of (a) the outer loops are also always present.

Hence, the presence of the bottom surface does not qualitatively affect the flow in the x - y plane, that is the plane parallel to the bottom plate. Let us consider the flow in the x - z plane for the same two sets of parameters. Vector plots and schematic diagrams are shown in Fig. 3.17. It is clear that the flow here has changed due to the presence of the bottom surface.

Putting everything together, we can say that away from boundaries a single

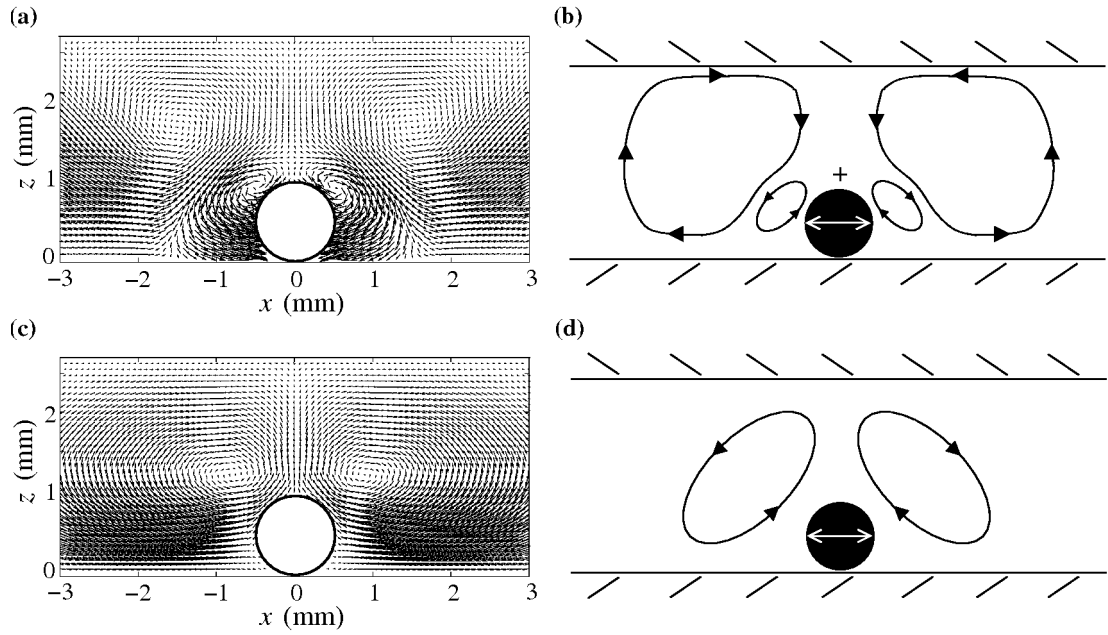


Fig. 3.17: Vector plot of the fluid flow for an oscillating sphere in a plane through the centre of the sphere. The axis of oscillation is the x -axis and the plane of the flow shown is the x - z plane. In (a) and (b): $Re=M^2=78.5$, $\epsilon=1.0$. In (c) and (d): $Re=25.4$, $M^2=6.7$, $\epsilon=3.8$.

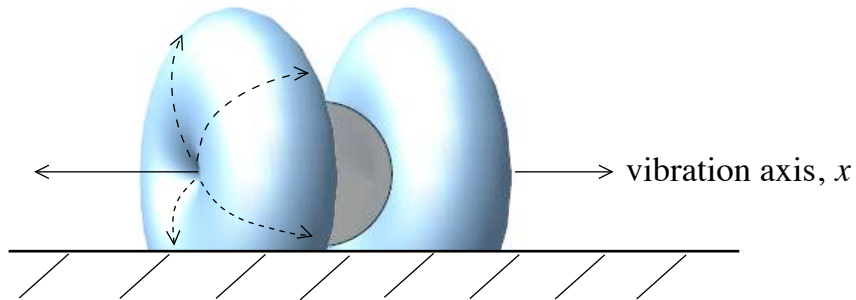


Fig. 3.18: Schematic diagram showing how the outer streaming flow is interrupted by the bottom surface. The sphere is oscillating along the vibration axis as indicated, generating a torus of fluid on either side. The presence of the lower surface cuts the flow so that the vortex loops are no longer closed but end on the surface.

oscillating sphere produces a three-dimensional fluid field around it which has rotational symmetry about the axis of oscillation, here the x -axis. The inner recirculation zone, formed near the surface of the oscillating particle, produces the outer recirculation zone which swirls in the opposite direction, see Figs. 3.3 (a) and 3.16 (a). As Re and M^2 decrease, the inner vorticity dominates, expands and diffuses away whilst the outer streaming is very weak, Figs. 3.3 (b) and 3.16 (b). With the presence of the bottom surface of the container, the rotational symmetry about the x -axis is interrupted and the streaming flow is cut almost halfway, as we can see in Fig. 3.17. Figs. 3.17 (a) and (b) show the vector plot of the average flow field round a sphere for $Re=M^2=78.5$, $\epsilon=1.0$, which corresponds to the same system as Figs. 3.3 (a) and Fig. 3.16 (a), but in the x - z plane. Similarly, Figs. 3.17 (c) and (d) show the vector plot of the average flow field round a sphere for $Re=25.4$, $M^2=6.7$, $\epsilon=3.8$, which corresponds to the same system as Figs. 3.3 (b) and Fig. 3.16 (b), but in the x - z plane. A three-dimensional representation of the flow near the lower surface is shown in Fig. 3.18.

3.5.2 Side boundary

Consider the flat boundary, plane B in Fig. 3.15, which is also parallel to the axis of oscillation but without the gravitational force affecting the motion. We shall investigate whether and how the sphere would interact with such a boundary. The reason will be more clear in the following chapters where the spheres will be free to move in a vibrated fluid-filled container.

Based on our understanding from the previous section, we expect that plane B will interrupt the streaming flow in the same way that plane A did, shown in Fig. 3.17. The modified asymmetric flow field may lead to a net force on the sphere because the difference here is that the sphere *can interact* with plane B.

We have run simulations measuring the time-averaged force on the oscillating sphere due to the presence of plane B as a function of the separation between the sphere and the wall, shown in Fig. 3.19. For higher Re , we find that the interaction force F_y is repulsive at small separations from the boundary and attractive at longer, slowly decaying to zero as the separation increases further. As

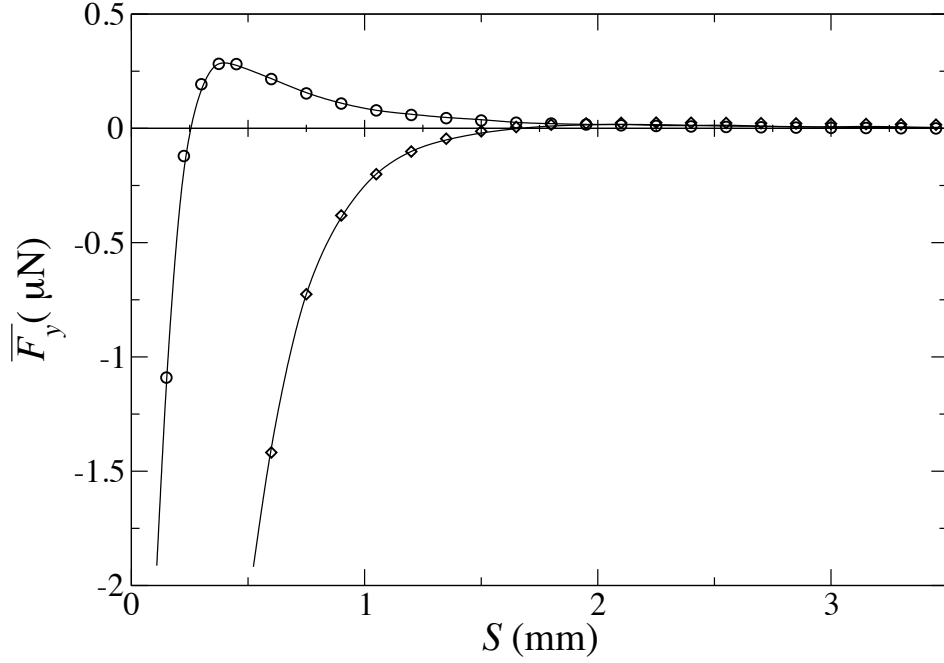


Fig. 3.19: The time-averaged interaction on a sphere oscillating near a wall parallel to it, as a function of the separation between the sphere and the boundary. $Re=M^2=78.5$, $\epsilon=1.0$ in circles and $Re=25.4$, $M^2=6.7$, $\epsilon=3.8$ in diamonds.

the Reynolds number decreases the force is predominantly repulsive slowly decaying to zero as the separation increases. This result is not completely surprising. Indeed there have been reports that when a single sphere is placed close to a boundary surface in the presence of an oscillating inviscid fluid flow, the sphere is attracted to the surface (Hassan *et al.* 2006a and b, Lyubimov *et al.* 2001) ; other workers have found both an attractive and a repulsive force depending upon the sphere-surface separation (Ivanova *et al.* 2005).

It is important to explain the way the average force F_y in the direction perpendicular to the oscillation is calculated; it is not straightforward as the drag force which is parallel to the direction of oscillation. Let us consider the parameters shown in Fig. 3.19 (circles), where $Re=78$, $f=50\text{Hz}$ and $\epsilon=1$. The instantaneous force F_y is shown in Fig. 3.20 in blue (circles) for a sphere-wall separation of 0.45mm . F_y is recorded every other time step, and in Fig. 3.20 it is plotted for an interval of one period $T=0.02\text{s}$, after 25 cycles of oscillation. For comparison we have also plotted, in red (squares), the drag force F_D , which is in the x -direction; F_D has been divided by 8 to fit on the same plot. The instantaneous force F_y fluctuates around $F_y=0$ and it is not clear what it would be like without

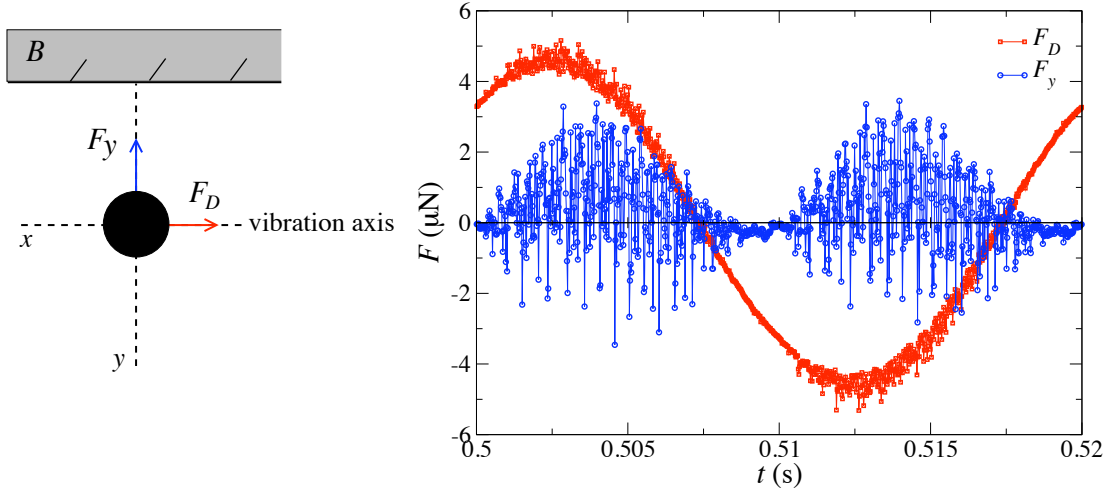


Fig. 3.20: Left: a schematic view in the x - y plane of a sphere oscillating near a wall B and parallel to it. The figure shows the orientation of the two forces acting on the sphere F_y due to boundary B , and the drag force F_D . Right: the forces F_y (blue circles) and F_D (red squares) are plotted against time for a fixed separation between the sphere and the boundary 0.45mm. The plot shows one cycle of oscillation of the sphere after 25 cycles.

the noise. The period of oscillation of F_y is twice that of the oscillation of the sphere. This is correct as the interaction force in the y -direction perpendicular to the axis of oscillation should not necessarily be aware of the positive and negative parts of the cycle of the sphere.

In order to tell whether there is a non-zero average of F_y we have to remove the noise first, by integrating F_y . We proceed as follows. For one cycle of oscillation of the sphere we integrate the force F_y using the trapezium rule, which is known to be a good estimate for the area under oscillatory functions. $F_y = F_y(t)$ is a function of time. The trapezium rule gives:

$$\int_a^b F_y(t) dt \approx \frac{b-a}{2n} (F_y(t_0) + 2F_y(t_1) + 2F_y(t_2) + \cdots + 2F_y(t_{n-1}) + F_y(t_n)) \quad (3.9)$$

where the interval $[a, b]$ is split into n smaller intervals. Here the first interval we consider will be $[a, b] = [0, T] = [0, 0.02]$. The number of the smaller intervals n is determined by the time step in the finite-difference calculation of the equations of motion and how often we have recorded the data, which here will be every other time step Dt . In other words, $f=50\text{Hz}$ and $Dt = 10^{-5}$, so we have $T/Dt=2000$ time steps per cycle. We record the force every other time step, so we have 1000 points per cycle. Therefore for the first calculation, $[a, b]=[0, 0.02]$ and $n=1000$. The trapezium rule is applied and we get an estimate of the force integral. We

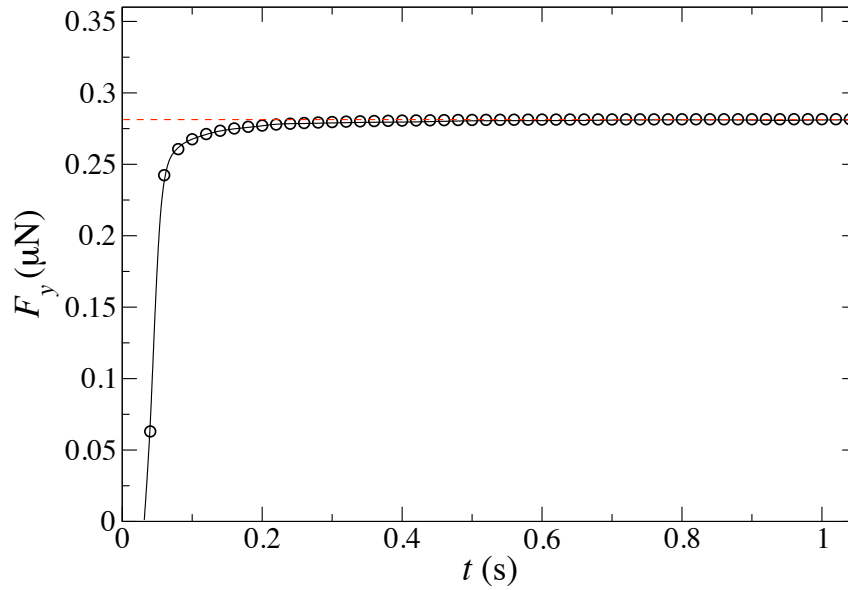


Fig. 3.21: The interaction force F_y for a separation 0.45mm between the sphere and the wall, after integration over many cycles, converges to an average value of $0.26\mu\text{N}$.

then multiply by T to get back the average force for the first cycle of oscillation. In this way we have obtained one value for the average force F_y for the first period of oscillation of the sphere. This process is repeated for many cycles, until steady state has been reached. The average force as a function of time is shown in Fig. 3.21. As we can see, it takes a few cycles for the force to stabilise but then it reaches a steady value. It is this value which corresponds to separation 0.45 mm between the wall and the sphere; it is one point in the graph of Fig. 3.19. This analysis is repeated for all the separations in order to obtain each of the two curves of Fig. 3.19 (corresponding to different parameters).

3.6 Discussion

In this chapter we have introduced some important concepts which will be met again in the following chapters. After a short introduction of oscillatory flow we focused on the case of a single sphere oscillating in a fluid. At intermediate Reynolds numbers this motion generates a non-zero time-averaged fluid flow called steady streaming. It is known that there are two structures of steady streaming which depend on the system parameters, shown in Fig. 3.3 (Riley 1966). Recent experiments (Kotas *et al.* 2007, Otto *et al.* 2008) which studied the three-dimensional flow field around a single oscillating sphere were discussed

and compared to our simulation results. We qualitatively validated our simulations against these experiments and other numerical studies (Chang and Maxey 1996, Alassar and Badr 1997). Our model is not extremely quantitatively accurate for the case of a single sphere. However, it does capture the behaviour of the system and it allows the addition of more than one spheres which can move freely as well as allowing them to interact with one another. This is the important feature of the computational method, because to the best of our knowledge, oscillatory systems with more than one interacting particles have not been simulated before. Towards the end of the chapter, we focus on the geometry and system parameters which we shall use in subsequent chapters. More specifically, we shall use a shallow fluid-filled container which is horizontally vibrated; the spheres sink to the bottom and then move with respect to the fluid once the vibration is switched on. We investigated how the flow field changes when a single sphere is brought near a surface and the interaction force between the sphere and the side walls of the container. The calculation of the interaction force between the sphere and the wall was described in detail. We are now able to computationally study the motion of more than one spheres. First, in the next chapter, we see what happens in experiment for two free spheres in an oscillating fluid flow.

Chapter 4

Two particle experiments

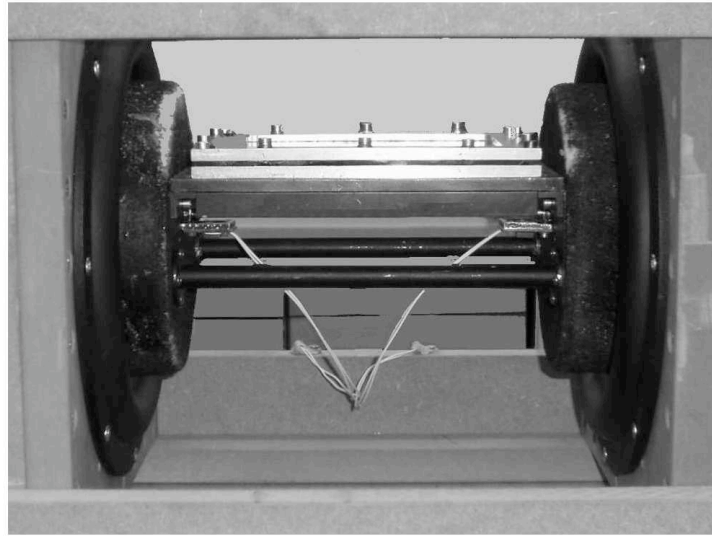
4.1 Experimental Details

In this chapter we describe a series of experiments aimed at understanding the interactions between two rigid spherical particles which were subjected to horizontal vibration in a fluid-filled container. The particles were found to align perpendicular to the axis of oscillation and sit with a gap between them. The details of this behaviour have been investigated. We have carried out experiments in which a pair of stainless steel spheres is shaken horizontally in a cell filled with glycerol/water fluid mixtures of three different viscosities, at various frequencies and amplitudes of oscillation. There is an equilibrium gap between the particles resulting from a long-range attraction and a short-range repulsion. The size of the gap was found to depend on the fluid viscosity and the vibratory parameters. We have identified two distinct scaling regimes for the dependence of the gap on the system parameters. First, the apparatus and the technical details for the conduction of the experiments will be described. Then the procedure, observations and results will be presented and discussed. In the next chapter the same system will be studied through simulations.

4.1.1 Vibratory Apparatus

The vibrational apparatus, shown in Fig. 4.1, consisted of a pair of electromagnetic transducers (eight-inch, Peerless, long-throw loudspeakers) mounted facing each other on a rigid medium density fibreboard, MDF, frame which was bolted

(a)



(b)

1. transducers
2. MDF frame
3. large concrete block
4. back MDF sheet
5. cooling tubes
6. metal plates
7. builders' foam
8. two rigid pillars
9. cell support metal frame
10. cell
11. accelerometers
12. high speed camera
13. resting board
14. small concrete blocks

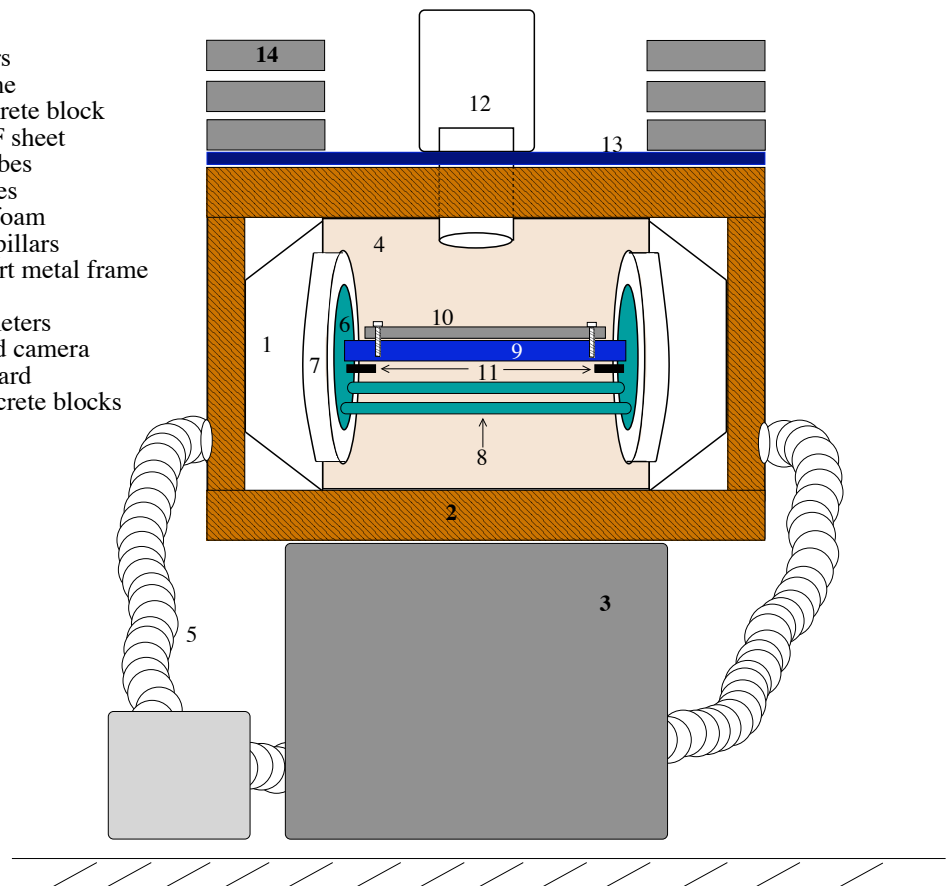


Fig. 4.1: The vibrational apparatus (a) a photograph and (b) a schematic diagramme with the components.

onto a large lead block, weighing $\approx 250\text{kg}$. The MDF kept the transducers fixed at their relative positions. An additional sheet of MDF was placed on one side of the apparatus in order to prevent potential twisting. The transducers were wired in anti-phase so that they moved in the same direction on application of a voltage. Two cooling tubes were constantly blowing air into the transducers to prevent overheating. A metal plate was attached to each transducer using expanded polyurethane foam so that it was perpendicular to the direction of oscillation. The two plates were connected through a rigid metal frame consisting of two pillars which ensured one-dimensional horizontal motion. Above the two pillars and parallel to them, also between the two plates, was the supporting metal frame on which the sample container was placed. The camera for capturing the motion was placed on a board resting on the top part of the MDF and held in place by small lead blocks weighing 1kg each. The one-dimensional motion of the transducers and, therefore the sample, was monitored using a pair of capacitance cantilever accelerometers, ADXL105 and ADXL150, attached to the transducers. These accelerometers covered the ranges $0\text{-}7\text{g}$ and $0\text{-}70\text{g}$ respectively. The output from each accelerometer passed through a 4-pole low-pass Bessel filter having a cut-off frequency of approximately 800 Hz . The Bessel filter was calibrated so the output shown on the digital voltmeter displayed the maximum acceleration of the transducers, Γ , directly for sinusoidal vibration. The control parameter for the experiments is the dimensionless acceleration, Γ , defined as

$$\Gamma = \frac{A\omega^2}{g}, \quad (4.1)$$

where A is the driving amplitude, ω is the angular frequency ($\omega=2\pi f$) and g is the acceleration due to gravity. A continuous sinusoidal waveform of the desired frequency was generated using a Stanford Research Systems DS345 signal generator. Signals of frequency, f in the range $10\text{-}100\text{ Hz}$ and peak-to-peak amplitudes of up to 1V were used during the experiments. The signal generator produced a sinusoidal waveform which was sent to an amplifier (Picker International, Gradient Drive Amplifier) passing through an on/off switch and a potentiometer which was used to control Γ . The output signal from the amplifier was fed back to the transducers. An oscilloscope (Hameg Instruments, Analog Oscilloscope, 35MHz ,

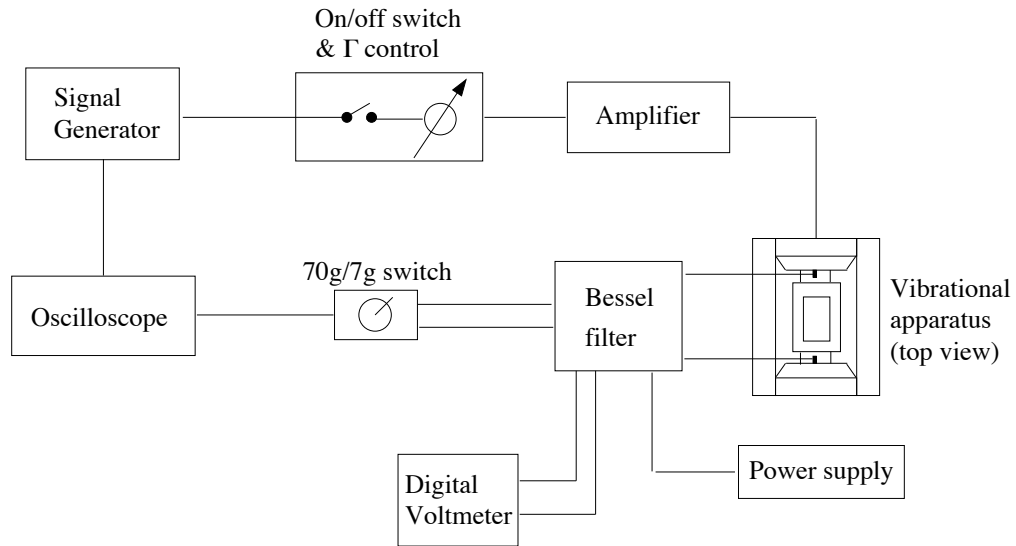


Fig. 4.2: A schematic diagram of the electronics of the apparatus.

HM303-6) was set up to show both the output from the Bessel filter and the output from the signal generator. The oscilloscope readings were used to ensure that the signal from the transducer was sinusoidal.

A photograph and a schematic diagram of the apparatus are shown in Figure 4.1. The connections of the electronic devices are shown in a schematic representation in Figure 4.2. Before every experiment the horizontality of the equipment was checked using an accurate spirit level.

4.1.2 Container

In all our experiments we used a liquid-filled cell formed by two 3mm thick glass sheets. Each sheet was glued into an aluminium alloy frame. The alloy was dural, which consists of 95% aluminium, 4% copper and 1% magnesium, making it strong but lightweight. The two frames were separated by a butyl rubber gasket to form a liquid-tight cell 135mm long and 95mm wide. The uniform spacing between the glass sheets could be varied but was set at 3mm in the majority of the experiments reported below. The cell was held together by ten screws which also passed through the rubber. Another four screw holes were cut so that the cell would be attached onto the vibratory apparatus. Two more holes allowed the liquid to be inserted into the cell and were fastened by two small screws and rubber washers. A schematic diagram of the container is shown in Fig. 4.3.

Depending on the measurements, we stuck some graph paper on the outside

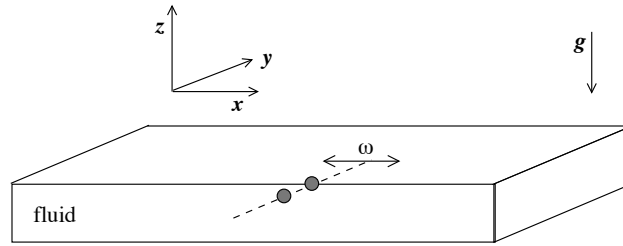


Fig. 4.3: A schematic diagram of the experimental cell. The three axes x , y , z are indicated, as well as the direction of the gravitational acceleration g and the axis of oscillation ω .

of the bottom glass sheet facing upwards, so that the graph paper could be seen from the top, under the spheres. This was done using Scotch Spray Mount Adhesive. The graph paper was needed in order to calibrate the distances which were measured when analysing images.

4.1.3 Fluid preparation

The experiments have been conducted using three different glycerol/water mixtures having kinematic viscosities $\nu = 2.0 \times 10^{-6} \text{m}^2 \text{s}^{-1}$, $4.5 \times 10^{-6} \text{m}^2 \text{s}^{-1}$, and $9.4 \times 10^{-6} \text{m}^2 \text{s}^{-1}$. For some experiments, when fluid visualisation was required, marker particles were added to the solution (Kalliroscope). Kalliroscope is a fluid used for that purpose; its viscosity is that of water $\nu = 1.0 \times 10^{-6} \text{m}^2 \text{s}^{-1}$. The concentrations of the glycerol percentage by weight in order for the fluid to have these viscosities, at $T = 20^\circ \text{C}$, along with the corresponding densities, are shown in Table 4.1.

Table 4.1: Viscosity and density of aqueous glycerol solutions at $T = 20^\circ \text{C}$.

Glycerol	Viscosity	Density
%weight	$\nu \text{ (m}^2 \text{s}^{-1}\text{)}$	$\rho \text{ (kgm}^{-3}\text{)}$
23.2	2.0×10^{-6}	1054.65
43.4	4.5×10^{-6}	1108.00
57.1	9.4×10^{-6}	1145.55

The values were calculated using linear interpolation from standard viscosity tables found online (<http://www.dow.com/glycerine/resources/table18.htm>). Since the fluid viscosity is a strong function of temperature, the laboratory temperature had to be controlled. When small fluctuations occurred, the above concentrations were adjusted so that the viscosities were kept at the desired values. During

recording with the camera illumination was needed, so extra cooling was applied through fans directed at the vibrating cell.

The cell was then filled with the selected liquid and particles and sealed so that, ideally, no air was trapped in the cell. In order to avoid the formation of air bubbles in the cell, the liquid was pumped just prior to use using a rotary vacuum pump.

4.1.4 Particle preparation

In the majority of the experiments reported here the particles used were non-magnetic, stainless-steel spheres, 1mm in diameter and of density $\rho=7950\text{kg m}^{-3}$. An additional, magnetic, steel sphere (2mm in diameter) was also placed in the cell. This sphere could be moved using a magnet positioned close to one of the glass sheets so that the pair under investigation could be repositioned. For a small number of measurements we also used stainless steel spheres 2mm and 0.5mm in diameter.

4.1.5 Cameras

A Kodak EktaPro EM (up to 1000 f.p.s.) high speed camera was mounted directly above the cell (Fig. 4.1) and the motion of the spheres was displayed on a monitor and recorded over a few cycles. The short film was then transferred to a Windows PC through a USB cable, where open source software “Pryme” was used to view and save each frame of the cycle as a separate image. Each image could then be analysed separately. Using different lenses, adjustments could be made to ensure as accurate a measurement as possible.

4.1.6 Procedure

Every time an experiment was conducted, the particles were cleaned with ethanol and dried. They were then placed on the bottom glass sheet of the cell along with the magnetic sphere. Then the rubber and top glass sheet were placed and screwed in, holding the cell together. The two holes used for filling the cell with liquid were not sealed yet. A syringe was used to transfer the selected liquid

from a beaker into the cell through one of these holes. Once the cell was filled, we tried to avoid the formation of bubbles by overfilling the cell, so that the air would come out. The cell was then sealed with two o-rings and screws. The cell was then attached onto the vibratory apparatus and the system was ready for measurements to be made.

In early experiments, small air bubbles formed in the cell under vigorous vibration. Their presence enabled us to observe that the spheres do not roll appreciably during vibration, since the attached air bubbles maintain the same orientation with respect to the cell. This observation is in agreement with the calculations of Wunenburger *et al.* (2002) who concluded that, under oscillatory liquid flow, spheres slip on the bottom of the cell rather than roll. Since the source of these air-bubbles was the air dissolved in the liquid, in the majority of our experiments the liquid was pumped just prior to use, using a rotary vacuum pump. Air bubbles did not then form.

4.2 Experimental Results

4.2.1 Preliminary Observations

Initially, a pair of spheres was placed in a liquid with $\nu = 2.0 \times 10^{-6} \text{m}^2 \text{s}^{-1}$. The frequency was 50Hz and $\Gamma = 5$. The spheres rapidly attracted each other as soon as the vibration began, moving to sit with a small gap between them, their line of centres being perpendicular to the oscillation. The variation in this gap during a vibration cycle was very small. During their motion the spheres remained very close to the lower glass sheet. The two spheres will only interact and move to this equilibrium configuration if they are initially placed sufficiently close to one another. If the vibration begins when they are in contact, they will repel one another and move to the same preferred configuration, a certain distance apart. Once a pair has formed, the two spheres oscillated in phase with one another in response to the driving amplitude. Because the spheres are not neutrally buoyant, their amplitude is smaller than the driving amplitude; they move with respect to both the vibrated cell and the fluid. As far as the motion of the spheres is concerned the relevant amplitude is that relative to the fluid, A_r . There will be

more discussion on relative amplitudes in section 4.2.5.

Wide-ranging measurements of the gap and the relative amplitude of the motion of the spheres with respect to the cell were conducted. In our experiments the cell was vibrated within the range of frequencies 10 - 70 Hz and within the range of Γ between 1 - 9, corresponding to a driving amplitude A in the range 0.2 - 6.6 mm. The parameter space that has been studied here is shown in Table 4.2.

Table 4.2: Experimental parameter space.

parameter	minimum	maximum
ν	$2 \times 10^{-6} \text{m}^2 \text{s}^{-1}$	$9.4 \times 10^{-6} \text{m}^2 \text{s}^{-1}$
f	15Hz	70Hz
A	0.2mm	6.6mm
Γ	1.0	9.0
ϵ	0.16	6.0
δ	0.103mm	0.315mm
Re	3	113
Re_s	0.7	403
M^2	5	84

Note that for low frequencies, sound waves are not excited so that the fluid can be treated as being *incompressible*. More specifically, the speed of sound in water is $v \simeq 1500 \text{ms}^{-1}$ and the container we use is $X=135 \text{mm}$ for its largest side. In order to get sound waves of comparable wavelength we would need to have frequencies of $f=v/X \simeq 10^4 \text{Hz}$. Our range of frequencies is between 10-70Hz which is a few orders of magnitude lower, and therefore we can assume we are operating in the incompressible flow regime.

For each frequency there is a range of values of Γ within which the interaction between the particles is strong and a stable gap may be observed. Below this range, the spheres may drift apart, usually at an oblique angle to the axis of oscillation, indicating that the interaction is too weak to hold them at right angles to the oscillation. If the spheres are very close to one another they may touch also at an oblique angle. As the upper end of the range of Γ is approached, the motion of the spheres becomes increasingly erratic and the gap fluctuates a

lot within a cycle. Beyond this upper limit the pair of spheres does not stay together.

The experiments were repeated many times using the more viscous fluids, with $\nu = 4.5 \times 10^{-6} \text{m}^2 \text{s}^{-1}$ and $9.4 \times 10^{-6} \text{m}^2 \text{s}^{-1}$. Experiments were also conducted in which the cell spacing was varied through the use of different thickness gaskets. It was found that the behaviour depended very little on the cell spacing provided that the spacing was at least twice the sphere diameter. In all of the experiments reported here this condition is met.

The reason for the alignment of the spheres perpendicular to the flow was not previously understood. Part of the aim of this chapter is to understand what regulates the equilibrium and why alignment is preferable. From our experimental observations it seems that if the spheres were aligned in the direction parallel to the flow, the configuration would be unstable. A possible explanation would be that when parallel to the flow the spheres experience unequal drag forces due to screening effects. However, a better understanding is required.

4.2.2 Image analysis

Both the equilibrium gaps and the relative amplitudes were extracted from the recorded images. An example is shown in Fig. 4.4. For the equilibrium gap, an image like this one was imported into *gimp* where the distance between the two particles was measured in pixels. The background graph paper (2mm side square) was used to convert the pixels into SI units. The procedure was repeated for a number of images so that the fluctuations in the gap were also taken into account. In order to measure the relative amplitudes of the spheres, we looked at consecutive images over a cycle and recorded the closest and the furthest distance of one of the spheres from a specific line (at right angles to the oscillation) on the background graph paper. The difference of the two distances gave the peak to peak relative amplitude of the particle with respect to the cell and therefore the fluid.

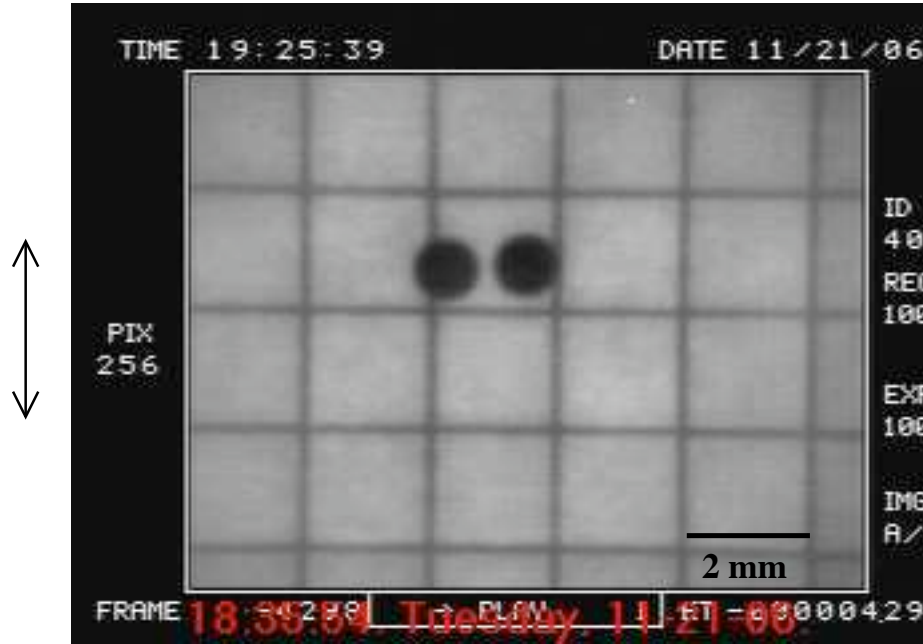


Fig. 4.4: An image taken from experiments showing two spheres forming a pair aligned perpendicular to the axis of oscillation, which is indicated by the double-arrowed line. The graph paper in the background is used to measure the relative amplitude of the spheres with respect to the cell.

4.2.3 Visualisation of fluid flow

The fluid movement induced by the spheres' motion could be inferred by observing marker particles. The movement consists principally of steady streaming flow. The form shown in Fig. 4.5 is typical: there is vigorous flow away from the spheres along the axis of vibration, the fluid returning along the orthogonal axis. The gap between the spheres is visible in the figure. Soon after the vibration is applied, fluid motion occurs close to the spheres. However, after a time of order of tens of seconds this flow extends to many times the sphere diameter, as is also clear from Fig. 4.6 (a)-(c).

It is also very interesting to note that the streaming flow around a single sphere looks similar in structure but is much weaker compared to that produced by the pair. We increased the contrast by illuminating the cell with stronger lights, shown in Fig. 4.7.

Although kalliroscope provides a way to get an idea of the structure of the flow field and its spatial extent experimentally, it is by no means an accurate method for making any kind of flow field measurements.

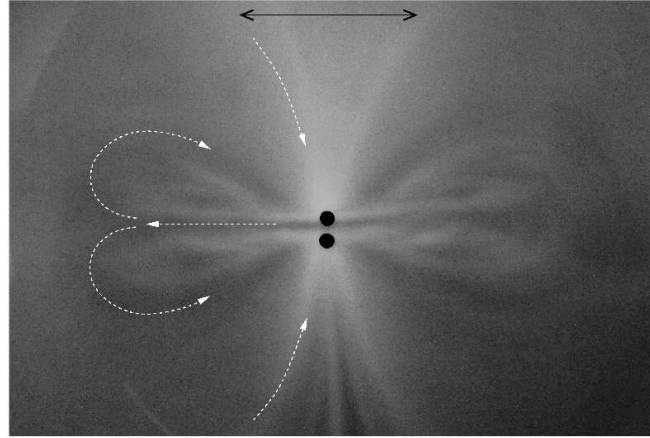


Fig. 4.5: The liquid flow patterns induced by a pair of 1mm diameter spheres, in a cell vibrated at 30Hz and with $\Gamma=6$. The liquid used was a glycerol and water mixture with $\nu = 2.0 \times 10^{-6} \text{m}^2 \text{s}^{-1}$. The white arrows indicate the direction of streaming flow on the upper side of the diagram, the flow on the lower side is the mirror image. The black, arrowed line indicates the direction of the oscillation.

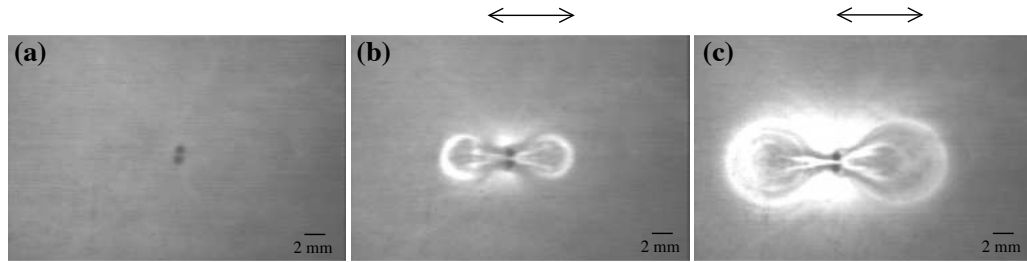


Fig. 4.6: The development of steady streaming for a pair of spheres oscillating in an oscillating liquid. (a) at $t=0\text{s}$ (b) $t=0.8\text{ms}$ (c) $t=2.16\text{ms}$

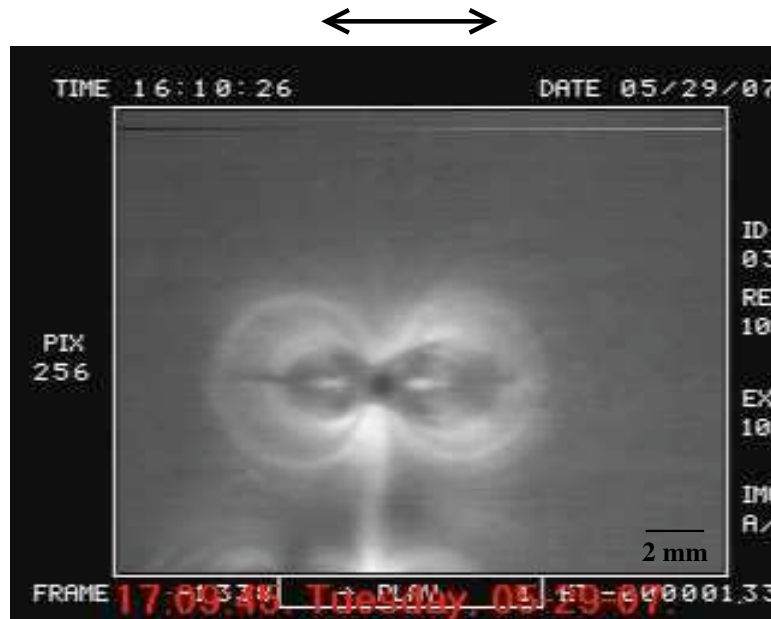


Fig. 4.7: The liquid flow patterns induced by a single sphere 1mm in diameter. The black, arrowed line indicates the direction of the oscillation.

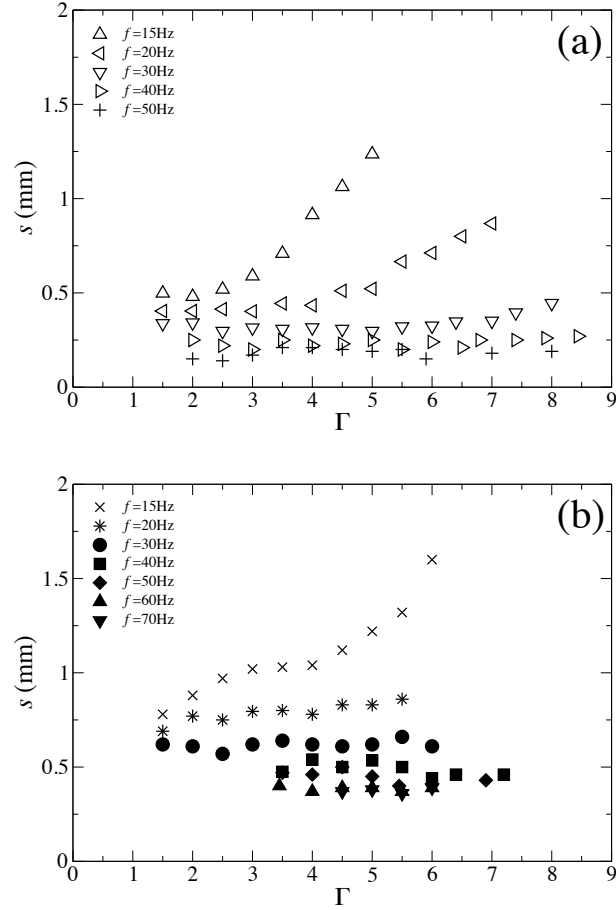


Fig. 4.8: The experimentally-determined equilibrium gap s between a pair of 1mm diameter spheres as a function of Γ for two different viscosities: (a) $\nu = 4.5 \times 10^{-6} \text{m}^2 \text{s}^{-1}$ and (b) $\nu = 9.4 \times 10^{-6} \text{m}^2 \text{s}^{-1}$ in (b). The frequencies used are shown in the legend. In these plots the scatter in the positions of the data points gives a good indication of the measurement errors.

4.2.4 Equilibrium gap

First we report the variation of the equilibrium gap, s , with Γ , f and ν . In Figs. 4.8 (a) and (b) we show how s depends on Γ , for $\nu = 4.5 \times 10^{-6} \text{m}^2 \text{s}^{-1}$ and for $\nu = 9.4 \times 10^{-6} \text{m}^2 \text{s}^{-1}$ respectively. It may be seen that, in each case, the gap grows rapidly with increasing Γ at low frequencies. The strength of this dependence gradually goes away as the frequency increases. Indeed, at the highest frequencies studied here, there is very little dependence of s upon Γ . There, the gap remains more or less constant.

For fixed Γ , the gap s drops with increasing frequency f , and the decay is more pronounced at higher Γ 's. At high frequencies, there seems to be little dependence of the gap on frequency.

The effect of viscosity is also evident as the two graphs Figs. 4.8 (a) and

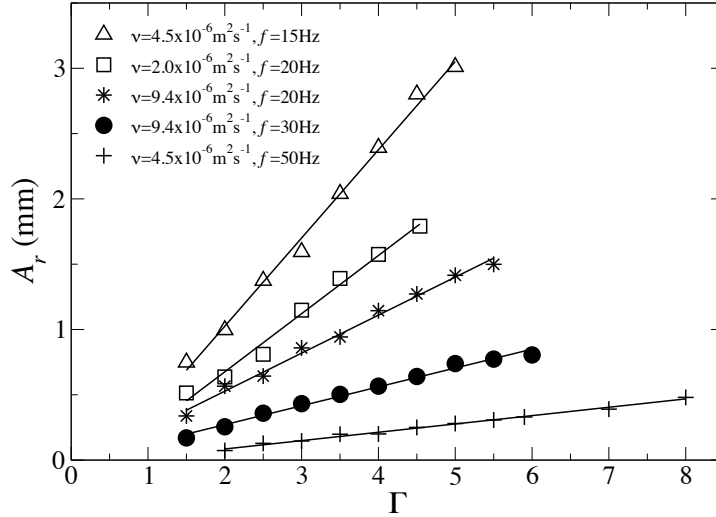


Fig. 4.9: The movement of the 1mm diameter spheres relative to the cell, A_r , plotted against Γ for various values of the viscosity and frequency. The lines shown are best linear fits to the data.

(b) differ. As ν increases, the range over which the gap depends strongly on Γ decreases. In other words, at high ν (Fig. 4.8 (b)) the gap depends strongly on Γ only for $f=15\text{Hz}$; for higher frequencies the gap is more or less constant. Whereas at lower ν (Fig. 4.8 (a)) the gap depends strongly on Γ for $f=15$ and $f=20\text{Hz}$. For each solution, there seems to be a threshold Γ at each frequency, which separates two regions, one with no gap dependency on Γ and one with a strong dependency on Γ . Note that in these figures the scatter in the positions of the data points gives a good indication of the measurement errors.

4.2.5 Relative amplitudes

When a cell full of liquid is subjected to vibration, the liquid moves with the cell because the liquid is incompressible. The spheres have a different density to the liquid so their inertia makes them oscillate with respect to the cell and also with respect to the fluid. In order to understand the motion of the spheres in detail, the *relative* amplitude of the spheres with respect to the cell, A_r , must be determined. For each of the viscosities used and the whole range of values of f and Γ , we have filmed a number of cycles of oscillation for a pair of spheres and, from the camera images, have determined A_r .

Figure 4.9 shows A_r plotted against Γ for some frequencies and viscosities shown in the legend. It may be seen that, in each case, the variation of A_r with

Γ is very close to linear, with no sign of curvature at upper values of Γ . However, the sphere only moves with respect to the liquid when a critical value of Γ is exceeded, this value depending somewhat upon ν and ω . The data may be fitted by the expression,

$$A_r = \frac{K(\nu, \omega)g}{\omega^2}[\Gamma - \Gamma_0(\nu, \omega)], \quad (4.2)$$

where $K(\nu, \omega)$ is a complicated function which varies slowly with ν and ω . The onset value, $\Gamma_0(\nu, \omega)$, lies typically in the range 0.2 -0.8: it has a low dependence upon the viscosity, ν , but increases with increasing ω . The presence of an onset and its frequency dependence have been considered in detail by Wunenburger *et al.* (2002) in terms of a model based on static friction and the viscous forces due to the translation and rotation of the sphere. Wunenburger *et al.*'s (2002) findings are consistent with our own observations. They conclude that for the values of Γ and ω considered here, each sphere slips across the surface rather than rolling upon it, for almost all of the vibration cycle. We confirm the lack of rotation in our own experiments by looking at small air bubbles trapped on a sphere's surface.

4.2.6 Data collapse

We saw that the equilibrium gap, s , between two spheres depends upon the frequency, f , the viscosity, ν , and upon the motion of the spheres relative to the cell, A_r . From additional experiments using spheres of diameters 0.5mm and 2mm we have also found that s is dependent upon the sphere diameter d . It is interesting to determine whether dimensionless ratios of these parameters may be used to collapse the data. The Reynolds number is a common choice, for fluid related systems. Specifically, for oscillating fluid flows, $Re = A_r \omega d / \nu$. In our parameter space Re ranges between about 5 and 120, a range intermediate between laminar flow and full turbulence, whereas the sphere size ranges over a factor of four and the viscosity and frequency each vary by a factor of five. If A_r is used to scale the gap and s/A_r is plotted versus Re we find that the data lies close to a single curve. This collapse is shown in Fig. 4.10. The same collapse plotted on a log-log scale is shown in Fig. 4.11. Most of the data lies reasonably

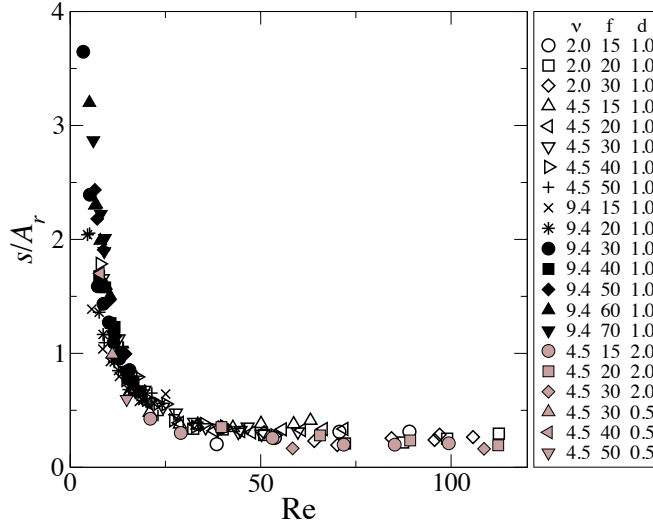


Fig. 4.10: The collapse of the experimental data when plotted as s/A_r against the Reynolds number, Re , for the various viscosities, frequencies and sphere diameters shown in the legend. In the table the viscosity ν is in units of $10^{-6} \text{ m}^2 \text{ s}^{-1}$, the frequency f is in Hertz and the sphere diameter, d , is in units of mm.

close to a line with a gradient of -1.0. This data may therefore be described approximately by the relationship

$$s = C\nu/(\omega d) \quad (4.3)$$

where C is a numerical constant. A fit using the value $C = 13$ is shown as the solid line in Fig. 4.12. It is noteworthy therefore that, for this data, the equilibrium separation does not depend upon A_r .

It may also be seen from Figure 4.11 that some of the data at higher values of Re do not scale in the way we have just described. The distinction between the two classes of data can be traced back to Figs. 4.8 (a) and (b). The data which undergoes the scaling collapse which we have just described, occurs for higher frequencies where the gap is not dependent upon Γ and thus upon A_r . However, these figures show that at the lowest frequencies, where A_r is large, the gap is extremely dependent both upon A_r and also upon frequency; the dependence upon A_r disappears very quickly as the frequency is raised. It is this lower frequency data, corresponding to the high Re data of Fig. 4.11, which does not undergo the scaling collapse just described. This data may be collapsed by plotting the gap, s , against $l = \frac{A_r}{d} \sqrt{\frac{\nu}{\omega}}$ as may be seen in Figure 4.13. On this log-log plot the collapse is close in form to a straight line with gradient of unity.

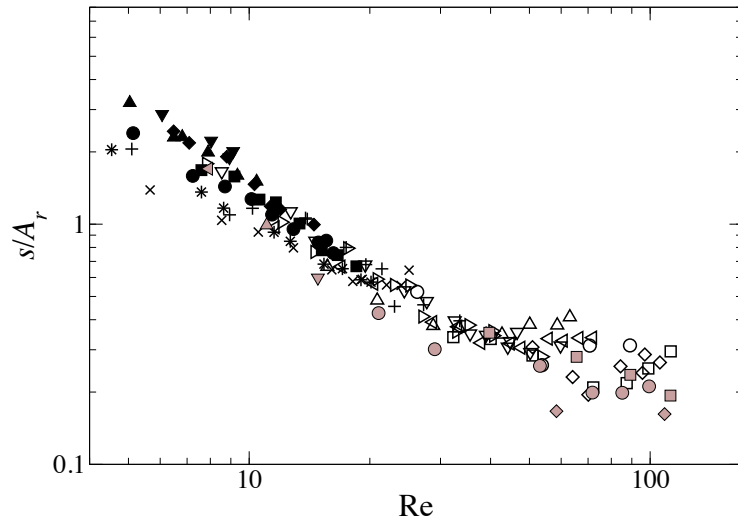


Fig. 4.11: The same data as in Fig. 4.10 plotted on a log-log scale.

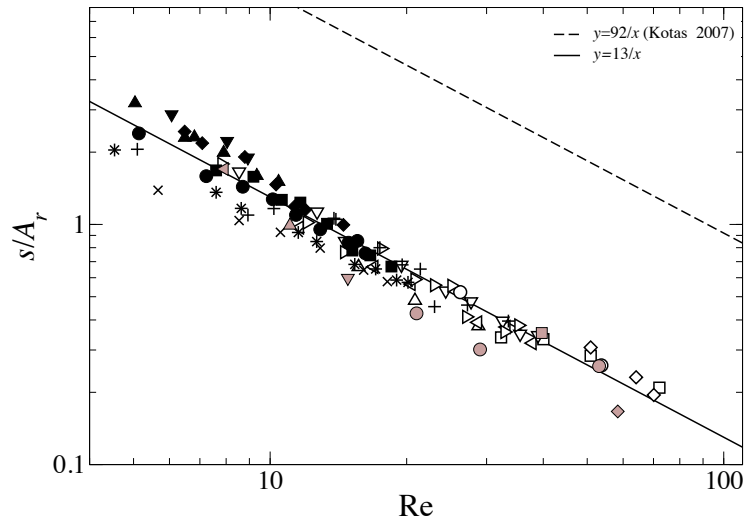


Fig. 4.12: The collapse of most of the experimental data shown in Figure 4.11, corresponding to the lower amplitude, lower Re limit. The scaled gap s/A_r is plotted against $Re = A_r \omega d / \nu$. The data can be fitted onto a curve $y = 13/x$ as shown. The dotted line further from the data points is the experimental collapse for the stagnation point distance from a single oscillating sphere found by Kotas *et al.* (2007).

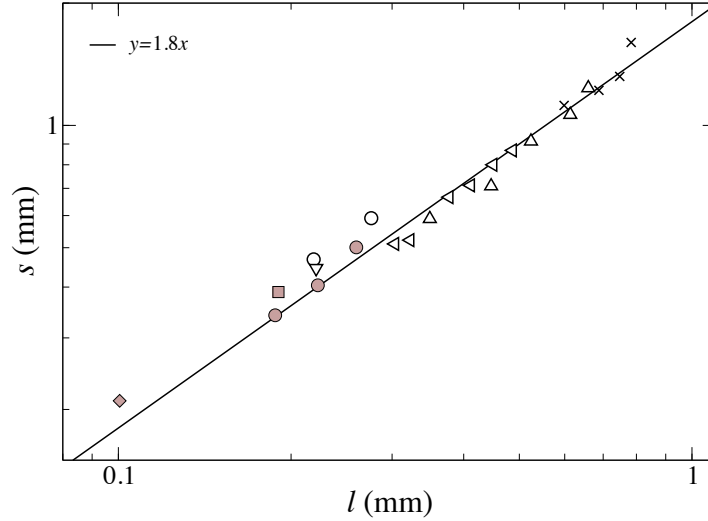


Fig. 4.13: The collapse of part of the experimental data shown in Figure 4.11, corresponding to the higher amplitude and higher Re limit. Here, the gap s is plotted versus $l = \frac{A_r}{d} \sqrt{\frac{\nu}{\omega}}$. The data can be fitted onto the line $y = 1.8x$ as shown.

For this data, therefore,

$$s \approx C' \frac{A_r}{d} \sqrt{\frac{\nu}{\omega}}, \quad (4.4)$$

where C' is a constant equal to 1.8 ± 0.2 . The cross-over from one form of scaling to the other is relatively abrupt. The condition for the cross-over may be obtained by equating the gaps in two scaling regimes. This gives the condition

$$A_r = \frac{C}{C'} \sqrt{\frac{\nu}{\omega}} \approx 7.2 \sqrt{\frac{\nu}{\omega}}. \quad (4.5)$$

We note that the length $(\nu/\omega)^{1/2}$ is the oscillatory boundary layer parameter associated with streaming flow (Batchelor 1967). Note that the symbols correspond to the same data sets for all these graphs, Figs. 4.10, 4.11, 4.12 and 4.13 shown in the legend of 4.10.

4.2.7 Discussion

We have shown that two spheres subjected to oscillatory fluid flow will attract each other and line up across the flow with a well-defined equilibrium gap between them. The existence of such an equilibrium configuration implies a long-range attraction and a short-range repulsion. Two distinct dependencies of the gap on the system parameters have been identified. Note that the ratio $\sqrt{\frac{\nu}{\omega}}$ is the

boundary layer thickness δ . At low amplitudes, we find that the gap depends on the square of the boundary layer divided by the particle size, $s \propto C\nu/\omega d$; at high amplitudes the gap depends on the boundary layer and amplitude divided by the particle size $s = C' \frac{A_r}{d} \sqrt{\frac{\nu}{\omega}}$. To the best of our knowledge both dependencies are new results which we published in Klotz *et al.* (2007).

Let us consider in more detail what happens in the low amplitude regime first, LAR. As the Reynolds number goes up and the boundary layer δ goes down, we move down the curve in Fig. 4.12 and the gap gets smaller. The collapse for this data is very interesting because the same dependence (with a different constant of proportionality) was found by Kotas *et al.* (2007) for the distance of the stagnation point from the surface of single oscillating spheroids. In Chapter 3 we briefly discussed the experiments conducted by Kotas *et al.* (2007); their scaling for the stagnation point distance T from single isolated oscillating spheroids obeyed $T \propto 46\nu/\omega d$, shown in Fig. 4.12 above our data collapse for the gap between two spheres. Note that the stagnation point here characterises the extent of the inner region flow, which is dominated by viscosity (Riley 1966). The fact that the equilibrium gap scales in the same way as the stagnation point distance, implies that the existence of a gap is also a viscous effect; in an inviscid flow where $\delta \rightarrow 0$ there would be no gap. This is consistent with our observations; as the Reynolds number increases and the boundary layer thickness δ goes down, Kotas *et al.* (2007) see the stagnation point distance from the surface moving in closer to the oscillating sphere and we see the gap between two oscillating spheres decrease. This could mean that the gap is nothing more than the boundary layer around each sphere which cannot completely overlap. Furthermore, remember that the two systems are quite different in terms of the experimental set up: in our experiments a pair of spheres slides on the bottom surface whereas in Kotas *et al.*'s (2007) experiments a single sphere is suspended in the middle of the container. The presence of the bottom surface in our experiments could affect the system in two ways: (i) it modifies the fluid flow so that in the vertical direction there is streaming above the sphere but not underneath, as shown in Fig. 3.17 from simulations in Chapter 3 for a single sphere; and (ii) it adds a frictional force on the spheres which are sliding on the bottom plate. The similarity in the

scaling behaviour between the suspended sphere in Kotas *et al.* (2007) and the pair of spheres in our experiments suggests that the effect of the bottom surface is secondary. For this reason, in our initial investigation we shall neglect the effect of friction and assume it is quite small compared to the dominant hydrodynamic forces. Nevertheless the presence of the bottom surface may be the reason for the difference in the constants C measured for the suspended sphere in Kotas *et al.* (2007) and the pair of spheres in our experiments

In the experiments of Voth *et al.* (2002), spheres were vibrated vertically in a viscous liquid ($\nu = 9.4 \times 10^{-6} \text{m}^2 \text{s}^{-1}$). Two types of interaction were identified perpendicular to the direction of oscillation: an attractive one, for which they suggested the secondary steady streaming flow as the source; and a repulsive interaction, which was not understood. In our experiments we also observed these two types of interaction, which lead to an equilibrium gap between the two spheres. If we are confident that the gap has a viscous origin, related to the stagnation point, then we can explain the repulsive force observed by Voth *et al.* (2002). Moreover, we can also explain the lack of a visible equilibrium gap in Wunenburger *et al.*'s (2002) experiments which were carried out in water (less viscous, $\nu = 1.0 \times 10^{-6} \text{m}^2 \text{s}^{-1}$).

Visualisation of the steady streaming flows between the two interacting spheres would greatly help our understanding. However, such an elaborate experiment would require optical techniques which we do not have. Only recently Otto *et al.* (2008) attempted to measure the streaming between two spheres using 3D Particle Image Velocimetry (3DPIV) but the details of the flow are difficult to distinguish. It would be a very interesting experiment to perform.

Let us now look at the high amplitude regime, HAR. The equilibrium gap scales in a different way to the stagnation point distance, as $s \sim \frac{A_r}{d} \sqrt{\frac{\nu}{\omega}}$; it becomes dependent on the relative amplitude and the boundary layer thickness $\delta = \sqrt{\frac{\nu}{\omega}}$, rather than δ^2 . This dependence kicks in when the amplitude of the spheres exceeds a cross-over value of $\sim 7\delta$. We have not found this scaling law in the literature. All the analytic studies make small amplitude approximations for the oscillating sphere. The experiments by Kotas *et al.* (2007) were also performed within the range of amplitudes that corresponds to the LAR in our

experiments. Otto *et al.* (2008) report a difference in scaling above a certain amplitude but their results are not conclusive. Andres and Ingard report a transition from one streaming flow to another through an amplitude increase. Riley says that difficulties due to separation of flow from the surface of the oscillating solid object arise in the low frequency, high amplitude case where $Re_s \gg \epsilon \gg 1$ which is the parameter space for the experiments in the high amplitude regime HAR. At this stage we do not know exactly why and how that cross-over in amplitude affects our system and whether separation of flow occurs.

In order to understand the details of these interactions we have carried out numerical simulations, described in the following chapter. Some of the immediate questions posed which we will aim to answer are the following. What do the fluid flows look like? How is the size of the equilibrium gap related to the fluid flow? What are the differences between the two scaling regimes? Can we measure the interaction force between the two spheres? Why is alignment perpendicular to the axis of oscillation preferred?

Chapter 5

Two particle simulations

In the previous chapter we described a series of experiments in which we found that there is an equilibrium gap between two macroscopic spheres oscillating in a viscous fluid, the spheres aligned perpendicular to the axis of oscillation. By investigating a parameter space at various frequencies, Γ 's and fluid viscosities, we found that there are two regimes for the gap scaling, depending on the amplitude of the spheres: the low amplitude regime (LAR), and the high amplitude regime (HAR). The scaling of the equilibrium gap in the LAR is the same as that of the stagnation point distance for a single isolated oscillating sphere (Kotas 2007). However, a number of questions arise: why is there an equilibrium gap in the first place? what is the source of the interaction between the two spheres? can we trace other differences between the two scaling regimes? why do the spheres align perpendicular to the oscillation?

We want to get more insight into the system to study features not readily accessible from experiment and to answer the above questions. With this in mind we have carried out a series of numerical simulations for two spheres. To the best of our knowledge no such simulations have been performed previously for oscillatory flows at intermediate Reynolds numbers.

The present chapter is organised in the following way. First we give details of the simulations. We then describe simulations for two spheres in a fluid-filled oscillating box and measure the equilibrium gaps, as we did in the experiments described in Chapter 4. The forces between two spheres along the line connecting their centres are then measured for various separations, under various conditions.

The fluid flow for both a single sphere and a pair of spheres at the equilibrium separation will then be presented and discussed. We then show the difference in the fluid flows between the extremes of the two scaling regimes. Placing the spheres off centre, we try to understand the mechanism for alignment by measuring the forces between two spheres at various positions relative to one another. The chapter ends with a short discussion.

5.1 Simulation details

The simulations were carried out using a time step $\Delta t = 10^{-6}$ s and a grid spacing $\Delta x = 7.5 \times 10^{-5}$ m to 1.0×10^{-4} m. In some of the simulations, we used a rectangular slab with dimensions $21\text{mm} \times 10.5\text{mm} \times 3\text{mm}$; in the rest we used a square slab with dimensions $21\text{mm} \times 21\text{mm} \times 3\text{mm}$ so as to study interactions between spheres kept far from walls.

The spheres are influenced by gravity in the vertical direction, aligned perpendicular to the largest faces of the container. As a result the spheres ride on the lower surface. However, to avoid the complications associated with lubrication forces, the spheres are prevented from reaching the outer cells of the fluid grid by a contact force which restrains them to be at least one lattice spacings from the true cell boundary. In Fig. 5.1 we show a snapshot demonstrating the geometry of the simulated system.

Three types of simulation have been performed: In the first, the system was chosen to model the experiments of the equilibrium gaps. The box and the fluid were oscillated and the spheres were free to respond to the oscillation. However, as we have not dealt fully with the interaction with the surface, which is known to be complex (Wunenburger *et al.* 2002), the simulated relative amplitude A_r is slightly higher than the experimentally measured value for a given set of driving conditions. In order to make a more direct comparison with experiment, while keeping the model computationally simple, we tuned the driving amplitude $A = g\Gamma/\omega^2$ so that the relative amplitude, A_r , of the spheres with respect to the fluid is the same as in experiments.

In the second type of simulation, the spheres were forced to oscillate sinu-

soidally with relative amplitude A_r with respect to the fluid, along x . Here, the fluid flows were generated by the motion of the spheres. The spheres were free to respond to the generated flows in the other two directions, y and z (but not the x -direction) and this is how the equilibrium gaps were measured.

In the third, for force and fluid flow measurements, the spheres were fixed at some constant relative position and were oscillated sinusoidally with relative amplitude A_r with respect to the fluid. Again, the fluid flow was generated by the motion of the spheres, but the spheres were always held in a fixed relative position to one another. Once the steady state had been reached (that is, the fluid velocities oscillated periodically at the driving frequency) the time-averaged forces on the spheres and the corresponding fluid flows could be determined. The type of simulation will be specified each time.

5.2 Equilibrium gap

Initially the fluid is at rest and the spheres are positioned across the cell at some separation their line of centres perpendicular to the axis of oscillation. While maintaining the walls of the cell at rest, both spheres are then oscillated along the longest horizontal dimension of the cell, x , as $A_r \sin(\omega t)$, using the experimentally measured values of A_r corresponding to the particular parameters being used. The fluid moves in response to the spheres' motion while the spheres are free to move without rotation, vertically and along the line joining their centres, under the influence of the fluid force, gravity and the surface contact force in the vertical direction. In practice we find little movement in the vertical direction, the spheres remaining one grid cell from the lower surface during their motion. Each simulation runs until a steady equilibrium gap is reached. A snapshot from simulation, using OpenGL, is shown in Figure 5.1.

In Figures 5.2 and 5.3 plots of the gap s between the two surfaces of the spheres versus time are shown for different driving conditions and fluid viscosities. It can be seen that the two spheres attract or repel depending on the parameters until they stabilise in their equilibrium positions, a certain distance apart, always kept perpendicular to the direction of oscillation. The equilibrium gap is reached

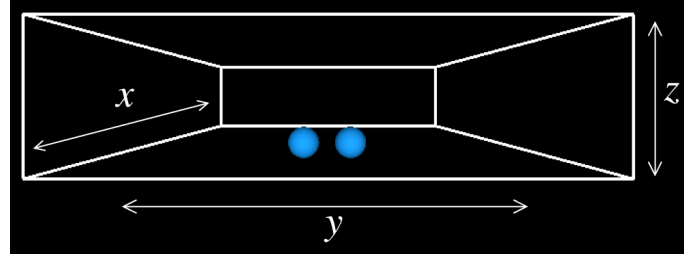


Fig. 5.1: Snapshot from simulation, showing two spheres at their equilibrium gap. Visualisation is achieved using OpenGL.

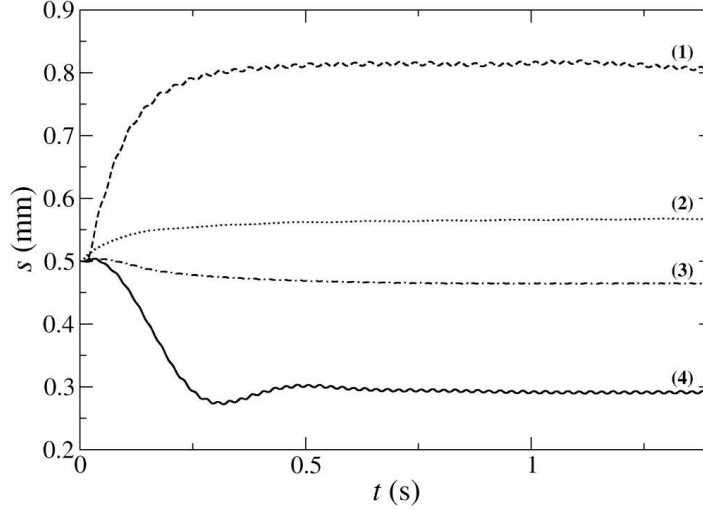


Fig. 5.2: The simulated gap versus time for parameters in the low amplitude regime, LAR. From top to bottom the parameters are: (1) $\nu=4.5 \times 10^{-6} \text{m}^2 \text{s}^{-1}$, $f=15 \text{Hz}$, $\Gamma=2.0$, $A_r=1.0 \text{mm}$, (2) $\nu=9.4 \times 10^{-6} \text{m}^2 \text{s}^{-1}$, $f=50 \text{Hz}$, $\Gamma=6.0$, $A_r=0.4 \text{mm}$, (3) $\nu=4.5 \times 10^{-6} \text{m}^2 \text{s}^{-1}$, $f=30 \text{Hz}$, $\Gamma=2.0$, $A_r=0.3 \text{mm}$, (4) $\nu=2.0 \times 10^{-6} \text{m}^2 \text{s}^{-1}$, $f=20 \text{Hz}$, $\Gamma=1.5$, $A_r=0.5 \text{mm}$.

within a time scale of order $< 0.5 \text{s}$ in most cases. However, we have checked that the equilibrium gaps remain unchanged over a total time of 8s.

The parameters used in the plot of Fig. 5.2 correspond more to the low amplitude regime LAR — see the caption for details. The spheres smoothly reach equilibrium, irrespective of whether that is closer or further out than their initial arrangement, which was a radius apart. In Fig. 5.3 we have plotted separations which would correspond to the high amplitude regime, HAR. Initially the spheres are repelled due to the instantaneous switching on of a high amplitude oscillation from rest. Equilibrium is reached in the same time scale, $< 0.5 \text{s}$ but the equilibrium gap fluctuates more than for the LAR in Fig. 5.2, an observation which is consistent with our experimental results which show that such fluctuations in the equilibrium gap between the spheres increase with amplitude.

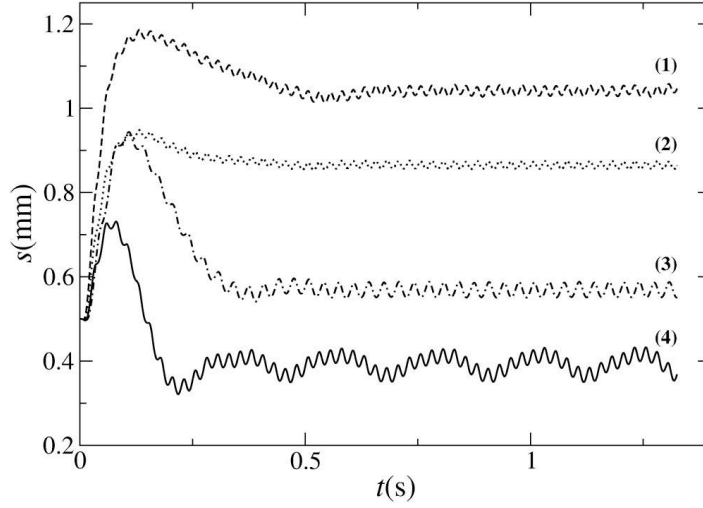


Fig. 5.3: The simulated gap versus time for parameters in the high amplitude regime, HAR. From top to bottom the parameters are: (1) $\nu=4.5\times 10^{-6}\text{m}^2\text{s}^{-1}$, $f=20\text{Hz}$, $\Gamma=6.0$, $A_r=2.18\text{mm}$, (2) $\nu=4.5\times 10^{-6}\text{m}^2\text{s}^{-1}$, $f=20\text{Hz}$, $\Gamma=5.0$, $A_r=1.71\text{mm}$, (3) $\nu=2.0\times 10^{-6}\text{m}^2\text{s}^{-1}$, $f=15\text{Hz}$, $\Gamma=3.0$, $A_r=1.89\text{mm}$, (4) $\nu=2.0\times 10^{-6}\text{m}^2\text{s}^{-1}$, $f=20\text{Hz}$, $\Gamma=4.0$, $A_r=1.58\text{mm}$.

We have carried out simulations for a large range of driving conditions and fluid viscosities. For each set of parameters the equilibrium gap is obtained after the steady state has been reached, from plots such as Figs. 5.2 and 5.3.

In order to compare with the experimental results of Chapter 4, we have analysed the data in the following way. Fig. 5.4 shows simulation data for the equilibrium gap, s , presented in the same way as the experimental data in Fig. 4.11. When plotted as s/A_r versus Re , on a log-log scale, the lower amplitude simulation data falls on a straight line with a gradient close to minus one. For this simulation data the constant C is close to 18 — see Fig. 5.5. As in experiment, the higher amplitude data scales differently, shown in Fig. 5.6. For this data the constant C' is close to 2.4. Both constants C and C' are somewhat higher in simulation than in experiment, which gave $C=13$ and $C'=1.8$. For comparison, the mean position of the experimental data is also shown in both figures as the dashed line. The transition from one scaling regime to another here occurs when

$$A_r \simeq 7.5 \sqrt{\frac{\nu}{\omega}} \quad . \quad (5.1)$$

The numerical constant ($\simeq 7.5$) for the cross-over is also slightly greater than the one from the experiments, which was $\simeq 7.2$.

We believe that the discrepancy between the simulated equilibrium gap data and the corresponding experimental data is partly due to the way we have treated

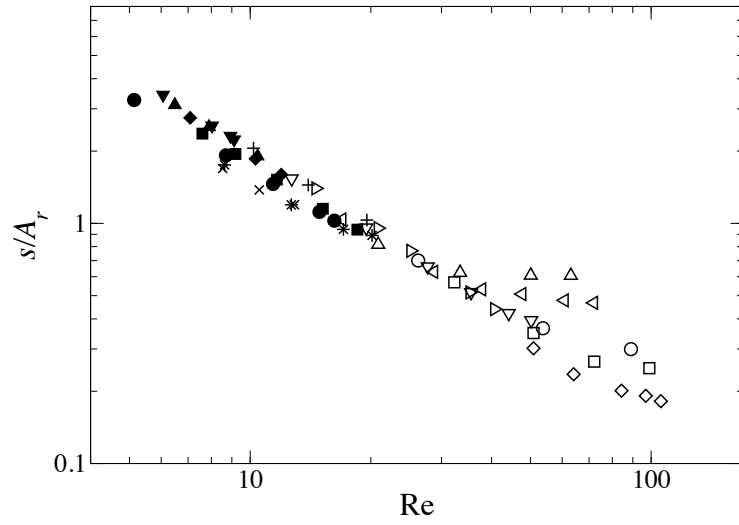


Fig. 5.4: Scaling collapse of the simulation data, presented in the same way as the experimental data shown in Fig. 4.11. The symbols correspond to the system parameters given in the legend to Fig. 4.10.

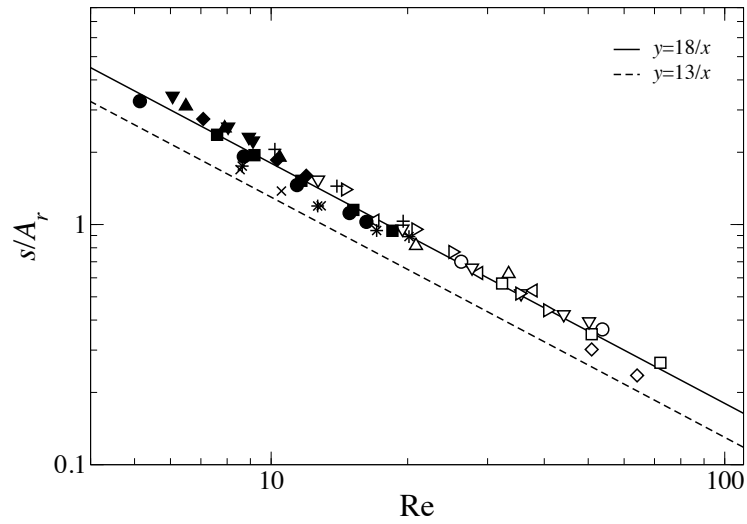


Fig. 5.5: The collapse for the lower amplitude data, LAR. The scaled gap s/A_r is plotted against $Re = A_r \omega d / \nu$. The data can be fitted onto a curve $y \simeq 18/x$ as shown in the solid line, which is higher than the experimental data collapse also shown in the dashed line.

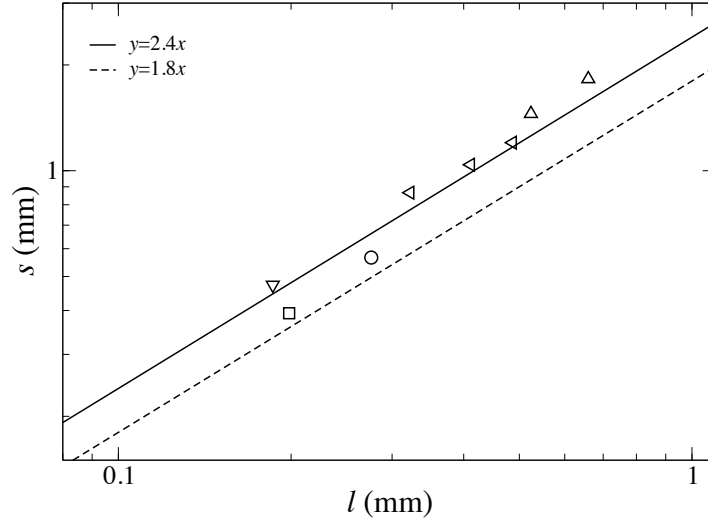


Fig. 5.6: The collapse for the higher amplitude data, HAR. The gap s is plotted against $l = \frac{A_r}{d} \sqrt{\frac{\nu}{\omega}}$. The data can be fitted onto a line $y \simeq 2.4x$ as shown in the solid line, which is higher than the experimental data $y \simeq 1.8x$ collapse also shown in the dashed line.

the interaction of the spheres with the surface and partly due to computational limitations. When the grid spacing is reduced further, the collapse curve for the simulated system shifts closer to the collapse of the experimental data, so better agreement is achieved. However, the finer the resolution the more computationally prohibitive the simulation becomes. For the same reason the simulated box is smaller than the one used in experiments. We cannot simulate a box as big as the experimental one using the required resolution because it would involve far too many points and would therefore be extremely time intensive. We have checked in simulation that varying the box size does not change the behaviour of the spheres. Nevertheless, it is clear that the simple model given here is able to capture, reasonably well, the main features of the experimental observations, giving us the confidence to use our model to investigate the fluid-driven mechanisms responsible for the gap.

5.3 Forces along the y -axis

Our aim here is to go into more detail about the interaction leading to an equilibrium gap between the two spheres. The presence of an equilibrium gap implies a short-range repulsion and a long-range attraction between the two spheres. The exact spatial range of this force and the magnitude are not known.

From simulation, it is possible to determine the forces on the spheres due to their motion with respect to the surrounding fluid. We consider the force on one sphere in the direction of the other, F_y , as a function of the spacing between between the closest surfaces of the two spheres, r_y . This can be obtained in the following way. The fluid is initially at rest and the spheres are positioned at a fixed separation. They are then oscillated in the direction perpendicular to the line joining their centres. The spheres are not allowed to respond to the flow, they only oscillate. The fluid flows are generated by the motion of the spheres. Once the steady state has been reached, the force on each sphere, $\mathbf{F}$, is calculated from

$$\mathbf{F} = \sum_i (-\nabla P + \nu \rho \nabla^2 \mathbf{v}), \quad (5.2)$$

where the sum is over all fluid sites occupied by a sphere and the derivatives are calculated using finite difference approximations. The details of the calculation of the time-averaged force were described in Chapter 3. The time-averaged force as a function of separation is shown in Figs. 5.8 and 5.7 for two typical sets of driving conditions. Here a positive value of F_y corresponds to an attraction and a negative value of F_y corresponds to a repulsion. The insets show the corresponding pressure force F_{py} and viscous force F_{vy} , the sum of which gives the measured force F_y , Equation (5.2).

As expected, at large separations the force is attractive whereas at small separations it is repulsive. The separation for which the force is zero corresponds to the equilibrium gap, s . The attraction peaks at $\simeq 0.3$ mm beyond the equilibrium gap, and then decays approximately as $r^{-\alpha}$. Unfortunately, it is very difficult to extract a consistent value for α from our data, but our best estimate is around 2.

From the insets, it can be seen that the shape of the pressure force is similar to that of the total force; it has a repulsive and an attractive part. The viscous force behaves in the same way but is much weaker. We have measured forces in this way for a range of parameters. From these force measurements, the only point we can make related to the two scaling regimes is that towards LAR the viscous force dominates making the overall force less and less attractive whereas in HAR the pressure force dominates, making the overall force less and less repulsive. In

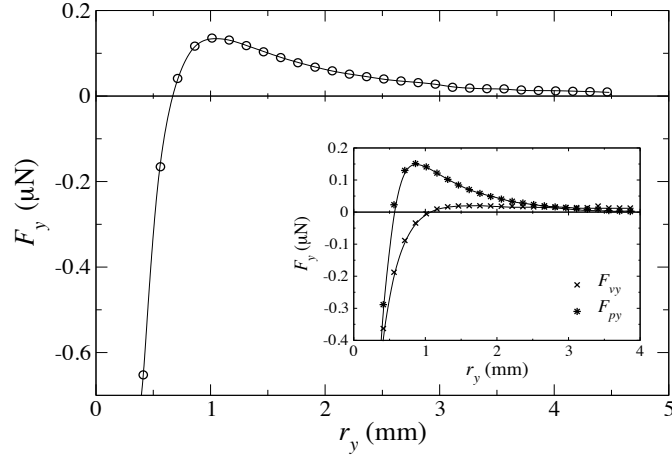


Fig. 5.7: The force F_y between two spheres in the direction perpendicular to the oscillation, as a function of the surface-surface separation r_y . The parameters correspond to regime LAR: $\nu=9.4\times 10^{-6}\text{m}^2\text{s}^{-1}$, $f=40\text{Hz}$, $\Gamma=6.0$, $A_r=0.57\text{mm}$. The inset shows the components of the force related to pressure F_{py} and viscosity F_{vy} .

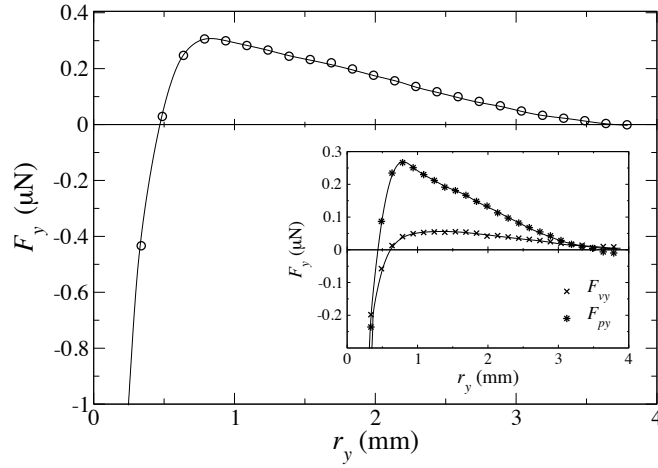


Fig. 5.8: The force F_y between two spheres in the direction perpendicular to the oscillation, as a function of the surface-surface separation r_y . The parameters correspond to regime HAR: $\nu=2.0\times 10^{-6}\text{m}^2\text{s}^{-1}$, $f=20\text{Hz}$, $\Gamma=4.5$, $A_r=1.79\text{mm}$. The inset shows the components of the force related to pressure F_{py} and viscosity F_{vy} .

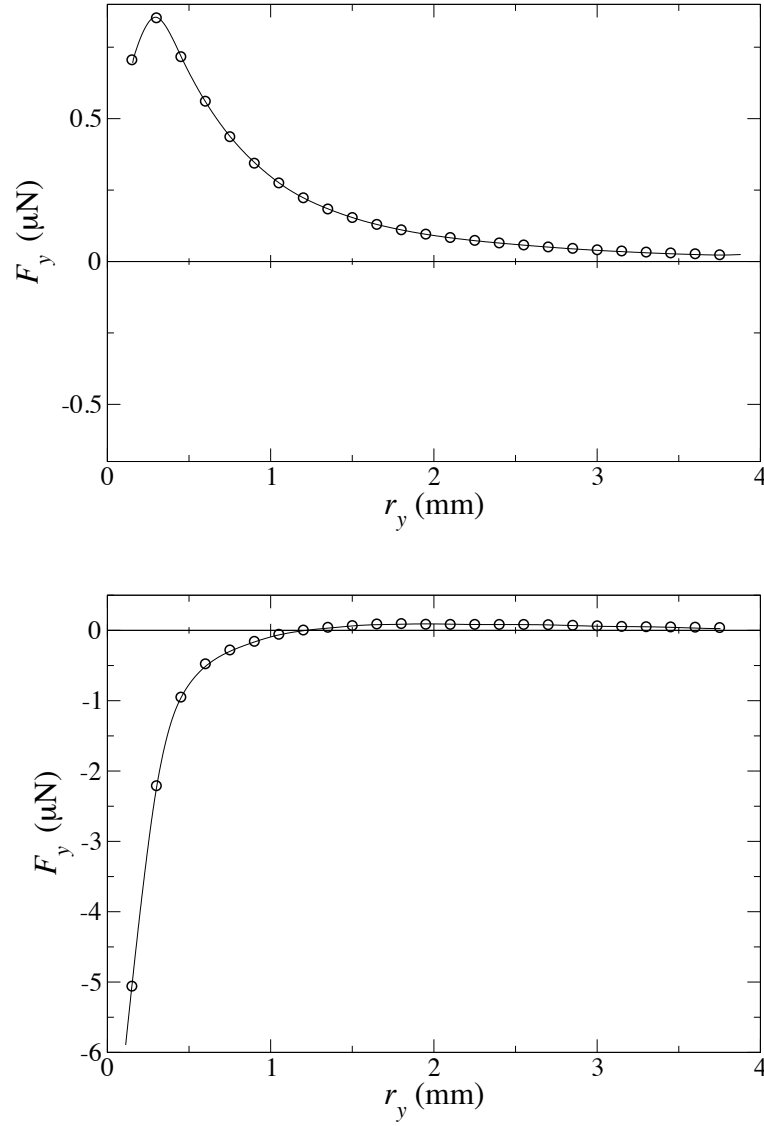


Fig. 5.9: The force F_y between two spheres in the direction perpendicular to the oscillation, as a function of the surface-surface separation r_y . Top: $\nu=2.0 \times 10^{-6} \text{m}^2 \text{s}^{-1}$, $f=50 \text{Hz}$, $\Gamma=5.0$, $A_r=0.5 \text{mm}$. Bottom: $\nu=4.5 \times 10^{-6} \text{m}^2 \text{s}^{-1}$, $f=15 \text{Hz}$, $\Gamma=2.0$, $A_r=2.21 \text{mm}$.

extremes of either regime, the force is found to be solely attractive Fig. 5.9 (top) or predominantly repulsive Fig. 5.9 (bottom).

The total force F_y shown here vanish at a separation which agrees with the equilibrium gap measurements from simulations when the spheres are free to respond even though the forces are time-averaged forces measured after the steady state has been reached, with the spheres oscillating in fixed relative positions.

5.4 Fluid flows at equilibrium

In order to understand the source of the forces which lead to the equilibrium gaps we shall turn our focus to steady streaming flows. We saw in Chapter 3 that there is a non-zero time-averaged fluid flow for an oscillating sphere at finite Reynolds numbers and we observed this effect from simulations for a single oscillating sphere. For two spheres we shall use the same model which allows us to determine the fluid flows generated by the motion of the spheres.

The spheres are held fixed at their equilibrium distance apart in y and are oscillated in x ; they are not free to move relative to one another. We consider the time-averaged streaming component of the flow, obtained by averaging the flow over one cycle of vibration once an equilibrium flow pattern has been reached. In simulation, the flow is generated by moving the spheres in a static box. However, for clarity, we will present the streaming flow field relative to the spheres.

First let us remind ourselves of the details of the steady streaming flow generated by one oscillating sphere. In Fig. 5.10 (a)-(b) we show the streaming flow for a single isolated sphere oscillating in a fluid with $\nu=2.0\times 10^{-6}\text{m}^2\text{s}^{-1}$ at $f=50\text{Hz}$ and $A_r=0.5\text{mm}$. The parameters are chosen as a typical example in the middle of our Re range in the LAR near the cross-over to the HAR. The sphere is oscillating along the x -axis. The flow shown is a slice taken through the centre of the sphere on the x - y plane.

In Fig.5.10 (a) the vector plot shown is taken from simulations and in (b) we have drawn a schematic diagram of (a) for clarity. The steady streaming flow for this isolated sphere qualitatively agrees with the theoretically predicted one, as we also saw in Chapter 3 (Riley 1966). There are four vortices near the surface of the sphere $\alpha - \alpha'$ on the left and $\beta - \beta'$ on the right. In absence of a bottom surface, there would be rotational symmetry about the axis of oscillation (x). Here the symmetry is broken due to the bottom surface and there is only partial rotational symmetry of the flow about x . Therefore vortices $\alpha - \alpha'$ are actually cross-sections of the same single vortex loop. Similarly $\beta - \beta'$ form another vortex loop around the sphere on the other side. The loop terminates at the bottom surface. (This may be clearer from the vector plot and schematic diagram of Fig. 5.11 (a) and (c) where the fluid flow in the x - z plane is shown.) Returning to

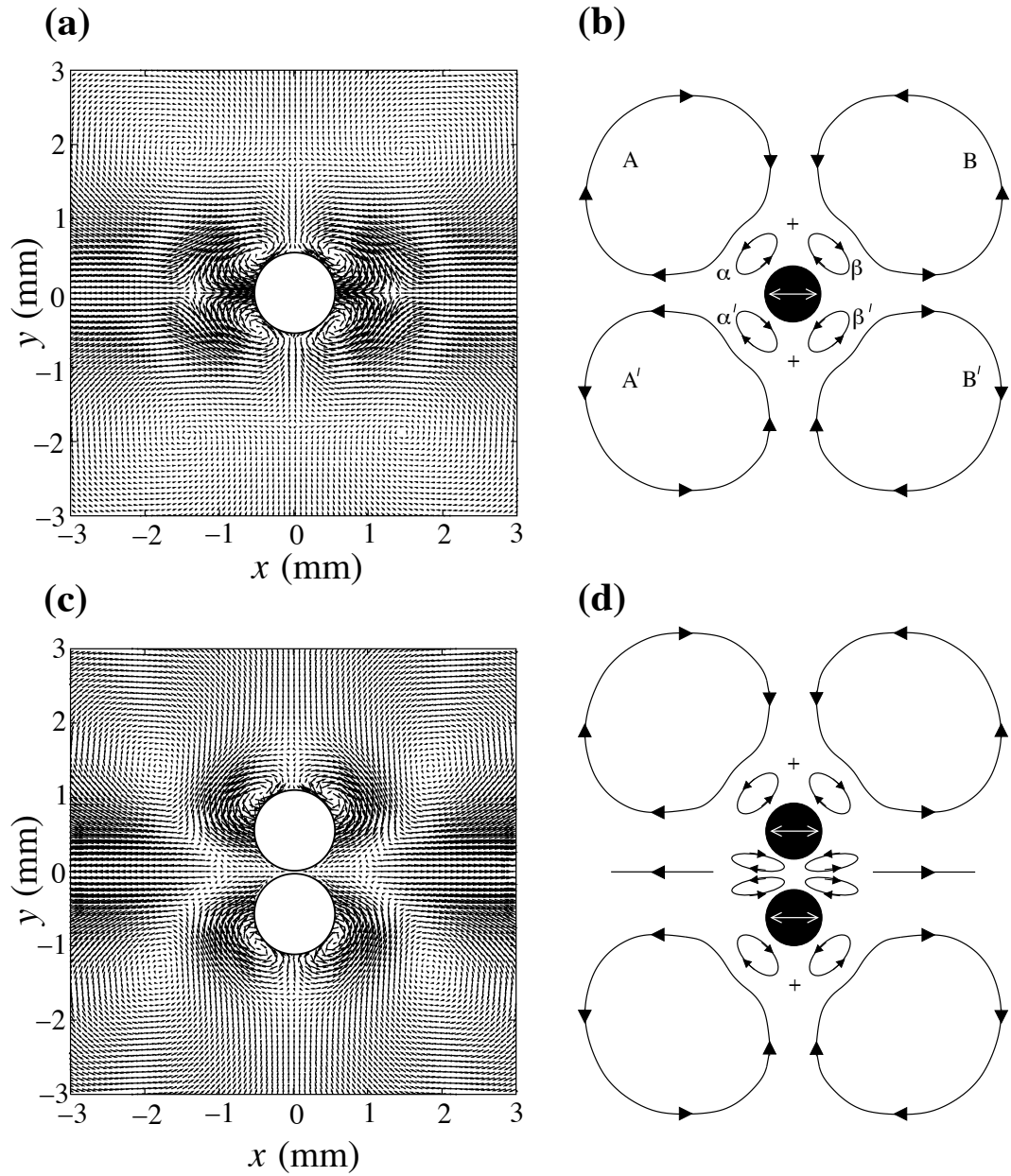


Fig. 5.10: The average streaming flow for a single isolated sphere (a)-(b) and for a pair of spheres at equilibrium (c)-(d). Vector plots taken from simulations are shown in (a) and (c) and the corresponding schematic diagrams are shown next to them (b) and (d). All simulations are done in a fluid with $\nu=2.0 \times 10^{-6} \text{m}^2 \text{s}^{-1}$ at $f=50 \text{Hz}$ and $A_r=0.5 \text{mm}$. The vectors in (a) have been scaled by the square of the distance from the centre of the sphere and in (b) by the square of the distance from the middle point between the two spheres.

Fig. 5.10 (a)-(b), the inner half torus on the left of the sphere, $\alpha - \alpha'$, gives a non-zero mean which disturbs the fluid further from the sphere creating another half torus circulating in the opposite direction, labelled A-A'. This outer vortex loop A-A' is spatially larger and weaker than the inner one. Similarly on the right of the sphere, there is an inner vortex loop $\beta - \beta'$ which drives the outer vortex loop B-B'. Around this one oscillating sphere, on average, there are *four* vortex loops. If we consider the flow on the $x-y$ plane only, shown in Fig. 5.10 (a)-(b) this is equivalent to *eight* vortices.

Let us now investigate what happens when, instead of the known streaming flow for one sphere, we have a pair of spheres oscillating at equilibrium, which is observed when two spheres are shaken in the vicinity of one another. In Fig. 5.10 (c)-(d) a vector plot and a schematic diagram for a pair of spheres at equilibrium are shown. Near the surface of each sphere there are four inner vortices, which are cross-sections of two vortex loops, same as before for a single sphere. In the region between the two spheres, the vortices are somewhat squashed due to the confined space, but are present nevertheless. However, there are only *four* outer vortices, rather than the eight which would be expected for two spheres in isolation. It seems as if the pair acts like a single sphere, a single object. The outer vortex pattern for the pair is qualitatively similar to that of a single sphere: it consists two outer vortex loops equivalent to four vortices in the $x-y$ plane. This result does not necessarily explain the existence of the equilibrium configuration, but it has shown us the vortex structure which is favoured when there are two spheres interacting.

More specifically, the outward flow is now centred on the gap rather than on the poles of the spheres. Because of the shift in the position of the outward flow, the circulation of the inner vortices within the gap strengthens this outward flow, resulting in strong jets of fluid flowing away from the gap. In (d) the two extra horizontal arrows illustrate the increased flow emerging from the gap between the spheres, in the plane of the spheres. This flow is part of the slightly elongated outer vortex loops, one on either side of the pair. It is as if, as the spheres are brought together, the overlapping streaming flows which have opposite circulation partially cancel, lowering the kinetic energy of the system. Once formed, a pair

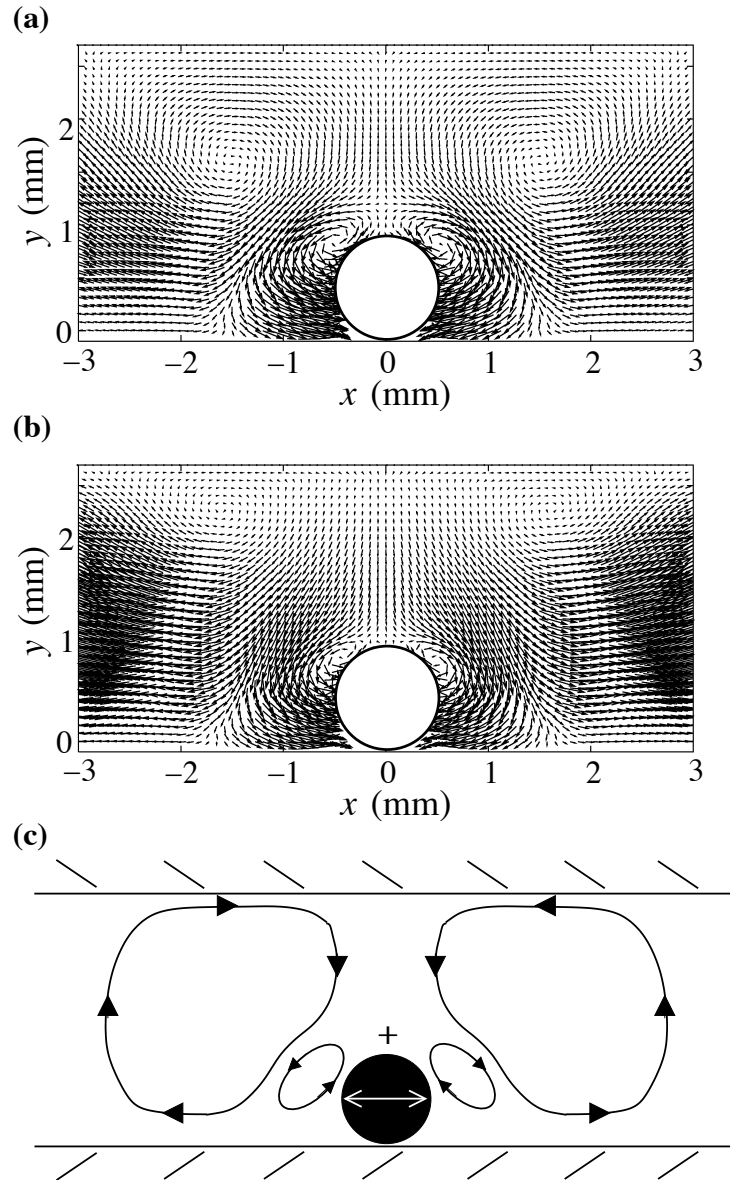


Fig. 5.11: The average streaming flow for a single isolated sphere (a) and for a pair of spheres at equilibrium (b). The vector plots are taken from simulations, through the centre of the sphere in the x - z plane in (a) and through the centre of one of the spheres in the x - z plane in (b).

of spheres is a very stable entity. The only experiments where the streaming flow of two spheres has been observed are those of Otto *et al.* (2008), which seem to agree with our simulations.

The presence of the bottom surface breaks the full rotational symmetry of the flow about the x -axis. What remains is approximately half of the flow generated by a single, isolated sphere. Figure 5.11 (a) shows a vector plot through the centre of the single sphere in the x - z plane. In Fig. 5.11 (b) a vector plot is shown through the centre of one of the spheres of the pair at equilibrium also in the x - z plane. Qualitatively the patterns are similar; in the case of the pair the outer flow is quantitatively stronger, because it is generated by a larger number of inner vortex loops and the eye of the vortex is shifted up in z . It can be seen that the streaming flow is similar to the flow that would have been generated in the half space $z > 0$, were the bottom surface not present. The vortex rings (inner and outer) terminate on the lower surface of the cell, forming open-ended vortex loops. A similar change in the fluid flow due to the presence of a surface has recently been observed experimentally (Otto *et al.* 2008). Figure 5.11 (c) is a schematic diagram of the flows shown in (a) and (b), included here for clarity. Note that the flow is somewhat squashed in the z -direction due to the top surface of the cell.

We also carried out simulations when the spheres are expected to be attracting each other (positioned further out than their equilibrium gap) and when they are expected to be repelling each other (positioned closer than their equilibrium gap). However, it is not straightforward to relate the forces to the average streaming flows. What we can say is that the further out the spheres are placed, the more they resemble two isolated spheres: each sphere has two inner and two outer vortex loops. When the spheres are held closer to one another, there is not enough space to accommodate the inner vortex loops in the region between the two spheres. Neither of these are equilibrium configurations.

5.5 Fluid flows from the LAR to the HAR

We have just seen the equilibrium flow generated by two interacting spheres. There are still unanswered questions. Why are there two scaling regimes for the equilibrium gap? Are there any differences between the extremes of the two types of equilibrium, one at low and one at high amplitudes?

In order to answer these questions we investigate the streaming flows of two sets of parameters corresponding to the extreme end of the LAR and the extreme end of the HAR: $\nu=9.4\times10^{-6}\text{m}^2\text{s}^{-1}$, $f=40\text{Hz}$, $\Gamma=6.0$, $A_r=0.93\text{mm}$ and $\nu=2.0\times10^{-6}\text{m}^2\text{s}^{-1}$, $f=20\text{Hz}$, $\Gamma=4.5$, $A_r=1.79\text{mm}$, respectively.

Figure 5.12 (a) and (b) show the time-averaged streaming flow for a pair of spheres in the LAR and the HAR respectively. These slices are taken through the centre of the spheres in the x - y plane, parallel to the lower surface of the container. In each case the sphere separation is fixed at its equilibrium value. At low amplitudes (Fig. 5.12 (a)), the flow is dominated by the eight inner vortices, close to the spheres. The flow around each sphere is similar in structure to that expected for a single sphere in isolation: near each sphere there are two inner vortex loops, or four vortices in the x - y plane. The vortices in the space of the gap are smaller and squashed compared to those on either side of each sphere. Riley (1966) has predicted that at very low $\text{Re}=A\omega d/\nu$ and $M^2=2r^2\omega/\nu$ (see Chapter 3 for more details) the inner vortices expand spatially and diffuse, whilst the outer streaming flow, the *secondary* flow gets weaker and weaker. In Fig. 5.12 (a), away from the particles the outer streaming flow is very weak indeed. We cannot see the secondary vortex loop at all. The inner vorticity is present and the viscous components dominate.

In contrast, at very high amplitudes, the dominant flow is associated with the outer vortices. The inner vortices here are spatially smaller and stronger. The eight inner vortices close to the spheres are still present. This picture is more like the one we described before for the modified flow for two spheres. Again we see that there are only four outer vortices, shown in Fig. 5.12 (b), rather than the eight which would be expected for two spheres in isolation. The outward flow from the gap is very strong. This behaviour has also been observed experimentally, as shown in Fig. 4.5 (Chapter 4). The outer flow is very far from the spheres

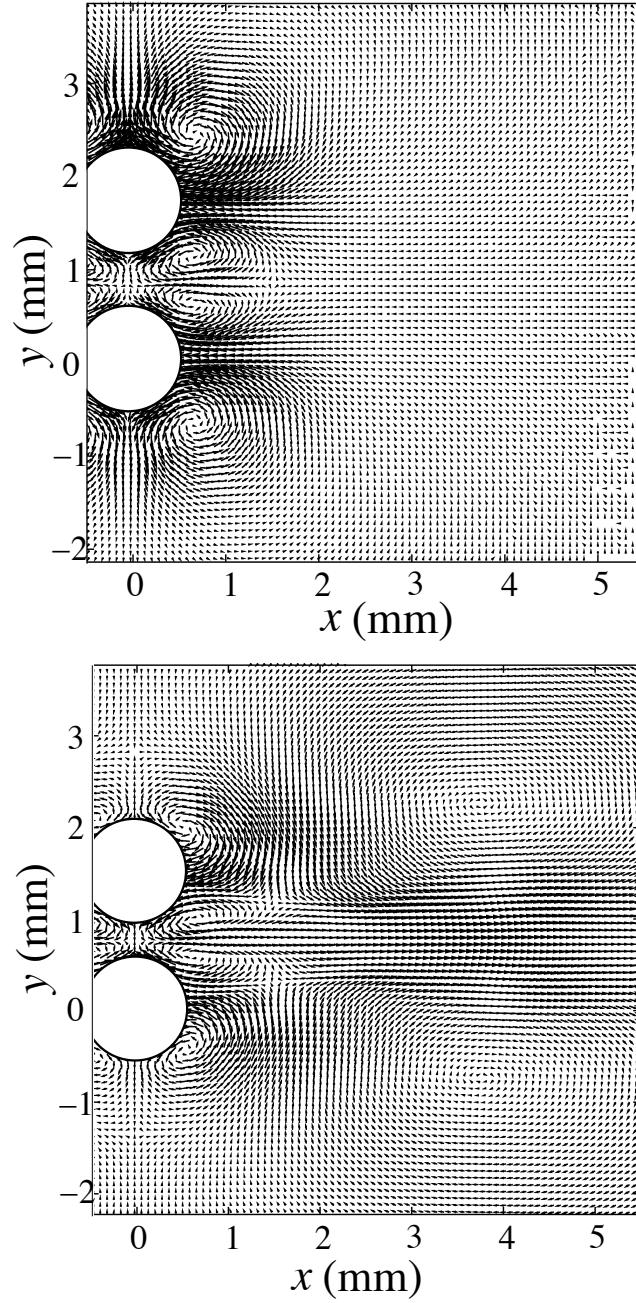


Fig. 5.12: Vector plots taken from numerical simulation of the average fluid flow for two 1mm spheres at their equilibrium gap. From top, the system parameters used are $\nu = 9.4 \times 10^{-6} \text{m}^2 \text{s}^{-1}$, $\Gamma = 6.0$, $f = 40 \text{Hz}$ and $\nu = 2.0 \times 10^{-6} \text{m}^2 \text{s}^{-1}$, $\Gamma = 4.5$, $f = 20 \text{Hz}$.

compared to Fig. 5.10 (c).

We have identified a difference between the two limits of the two scaling regimes. However, we must remember that in the presence of secondary streaming, the outer vortex structure generated by the inner vortex structure is not the sole characteristic of the high amplitude regime, HAR. We saw earlier, Fig. 5.10, secondary streaming develops in the LAR too. Really the defining line between the two regimes is not simply the generation of secondary streaming. In Fig. 5.12 (b) the outer streaming is stronger than in Fig. 5.10 (c) but, more importantly, there is another difference: it seems that the outer vorticity is much further from the particles.

Based on the two scaling regimes discovered experimentally in Chapter 4, the cross-over is amplitude-induced and occurs when $A_r \simeq 7.5\delta$. Note that for the same driving amplitude, the relative amplitude of the spheres is higher at lower viscosities, which is why most of our low amplitude data are taken for high ν and most of our high amplitude data for low ν . We should be able to see the transition from the LAR to the HAR for a certain set of parameters by increasing the amplitude only, keeping everything else the same. We have run simulations for $\nu = 4.5 \times 10^{-6} \text{m}^2 \text{s}^{-1}$ and $f = 20 \text{Hz}$, and a range of increasing Γ 's. The cross-over should occur when $A_r \simeq 1.42 \text{mm}$. In Fig. 5.13 we show vector plots for the time-averaged fluid flow for (a) $A_r = 0.61 \text{mm}$, (b) $A_r = 1.03 \text{mm}$, (c) $A_r = 1.36 \text{mm}$, and (d) $A_r = 2.58 \text{mm}$. The cross-over can be observed between (c) and (d) as expected.

We have tried to generalise the changes that take place when we go from one regime to the other, based on our results for the average streaming flow of various parameters at low, medium and high viscosities, frequencies and amplitudes. In Fig. 5.14 we have plotted a schematic diagram which illustrates this transition. More specifically Fig. 5.14 (a) shows the low-amplitude behaviour, the inner vortices close to the gap are relatively weak and there is a stagnation point nearby. As the amplitude increases, the inner vortices close to the gap increase in magnitude and spatial extent, and the stagnation point moves away. The resulting flow is shown in Fig. 5.14 (b). At yet higher amplitudes, the outflow from the gap is sufficiently strong to generate large outer vortices, as shown in

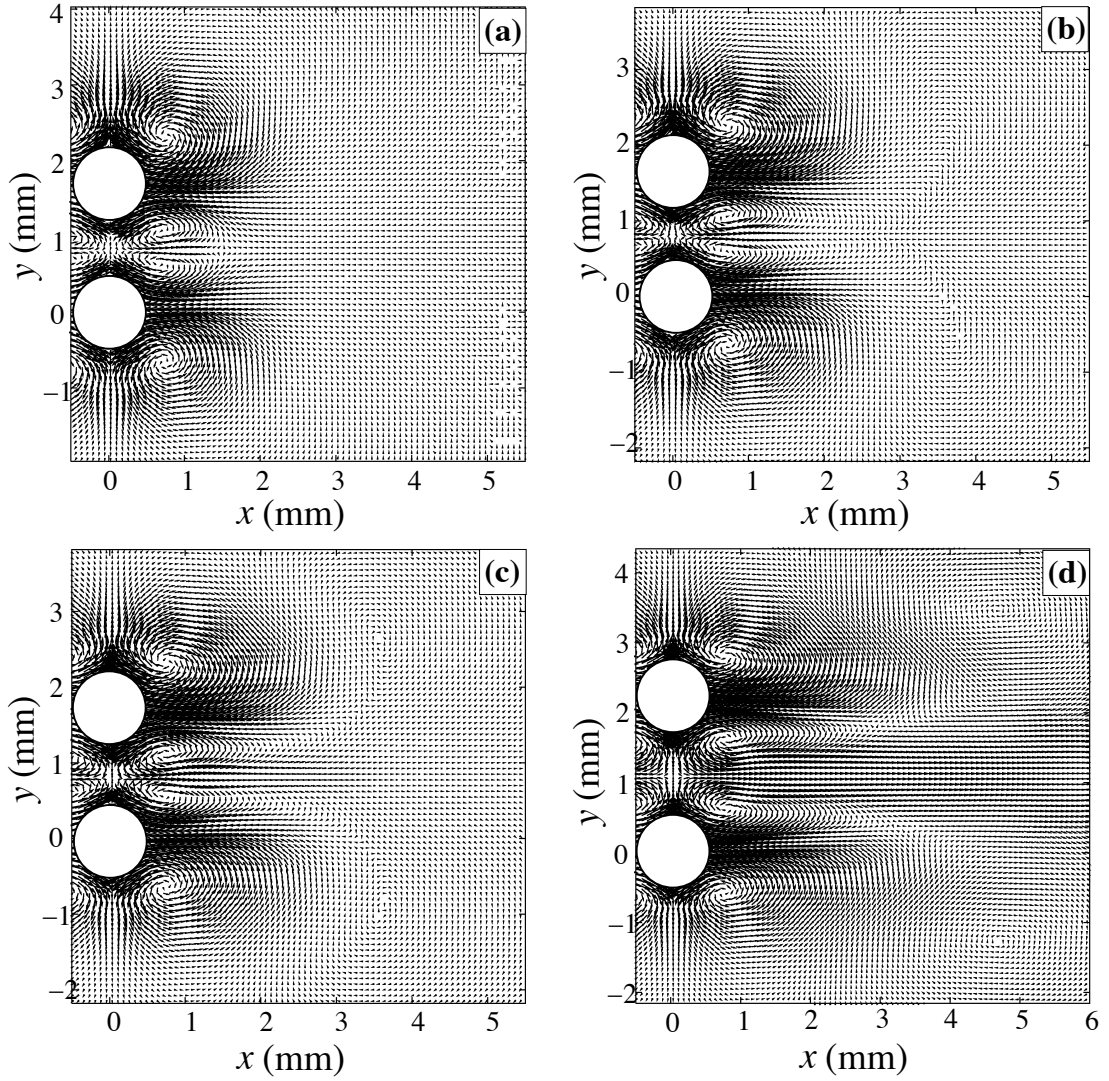


Fig. 5.13: Vector plot taken from numerical simulation of the average fluid flow for two 1mm spheres at their equilibrium gap for $\nu = 4.5 \times 10^{-6} \text{m}^2 \text{s}^{-1}$ and $f = 20 \text{Hz}$. The streaming flow changes from the LAR to the HAR as the amplitude of the spheres increases from (a) $A_r = 0.61 \text{mm}$, (b) $A_r = 1.03 \text{mm}$, (c) $A_r = 1.36 \text{mm}$, and (d) $A_r = 2.58 \text{mm}$.

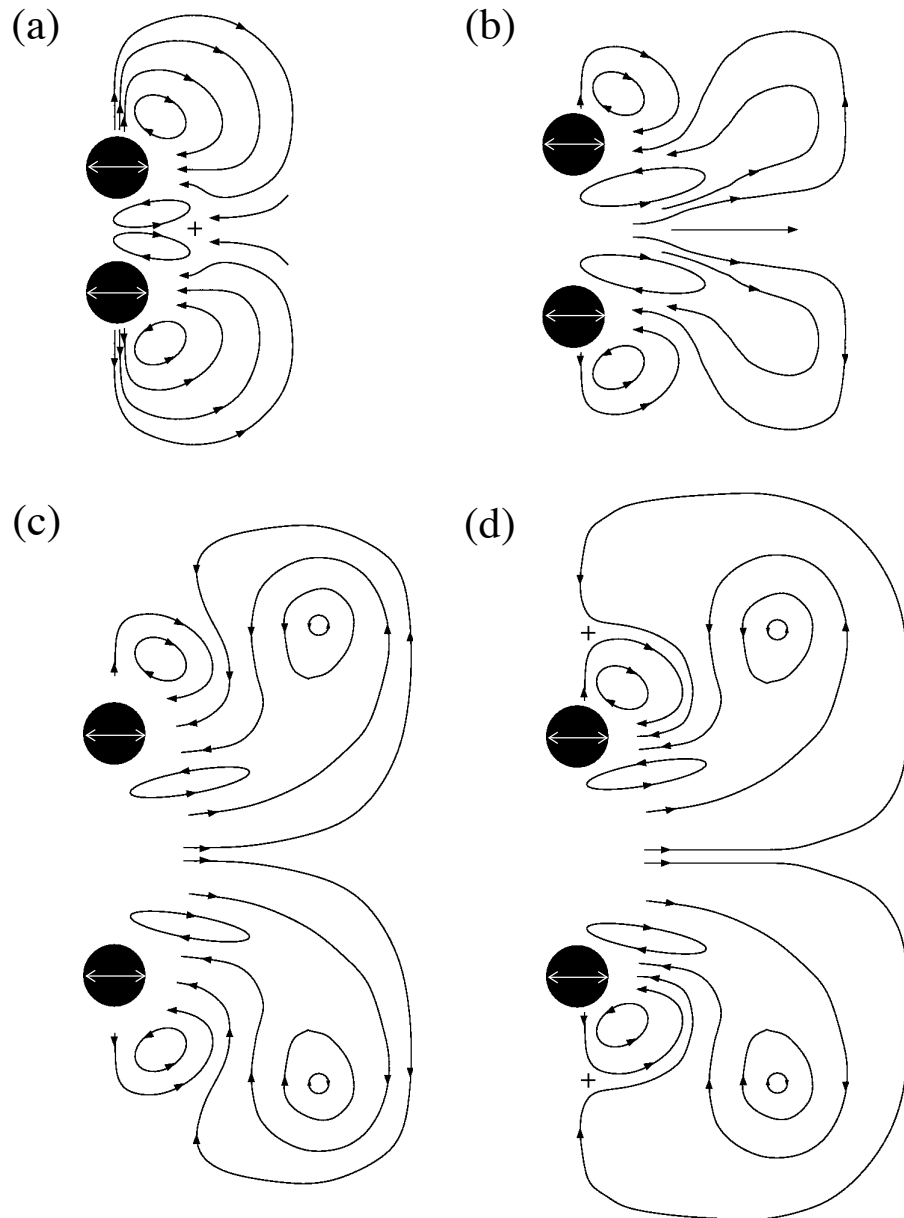


Fig. 5.14: Schematic diagram of the average fluid flows through the transition from the LAR to the HAR.

Fig. 5.14 (c) and (d). The outflow now can return along a line joining the centre of the spheres, until it approaches the stagnation point. As far as we can tell there is a smooth transition from one regime to the other.

5.6 Two-sphere alignment

We saw experimentally that when two spheres are placed in the vicinity of one another they rapidly align perpendicular to the vibration and sit at their equilibrium gap. This effect has been predicted theoretically for inviscid flows (Lyubimov *et al.* 2001), and observed experimentally in viscous flows as described in detail in Chapter 4 and also in (Wunenburger *et al.* 2002, Voth *et al.* 2002 and Klotz *et al.* 2007). In our simulations so far the spheres have always been aligned perpendicular to the oscillation from the beginning. It seems that the equilibrium configuration and the average flow favour the pair to be aligned this way, however in this section we shall try to understand more details about the alignment mechanism.

We will estimate the interaction force between two oscillating particles A and B whilst keeping their relative orientation and spacing constant. More specifically, particle A is placed in the centre of a square box and one grid point above the bottom surface. Particle B is then placed at some position relative to A in the same plane, as shown in Fig. 5.15. The fluid is initially at rest. The two spheres are then oscillated with the same amplitude in the x -direction keeping their relative position fixed. The time-averaged force on particle B is measured. The position of particle B is then varied and the process is repeated. In this way we obtain a vector plot showing the force on particle B at various orientations with respect to particle A. Figure 5.15 shows a vector plot of this force for $\nu=2.0\times10^{-6}\text{m}^2\text{s}^{-1}$, $f=50\text{Hz}$, $A_r=0.5\text{mm}$. The length of the arrows gives a measure of the strength of the force, acting on the centre of particle B. The simulations have been repeated for $\nu=4.5\times10^{-6}\text{m}^2\text{s}^{-1}$, $f=50\text{Hz}$, $A_r=0.4\text{mm}$ and $\nu=9.4\times10^{-6}\text{m}^2\text{s}^{-1}$, $f=30\text{Hz}$, $A_r=0.83\text{mm}$; force vector plots are shown for these sets of parameters in Figs. 5.16 (top) and (bottom) respectively.

By studying Fig. 5.15 we see that there is one stable position for particle B,

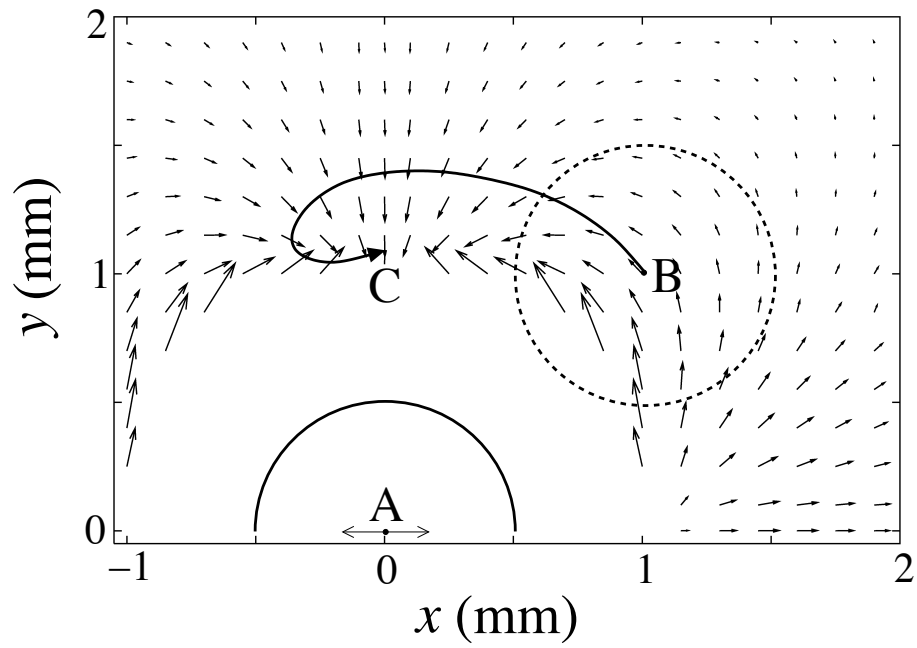


Fig. 5.15: Vector plot of the effective force acting at the centre of particle B placed near particle A, for $\nu=2.0\times10^{-6}\text{m}^2\text{s}^{-1}$, $f=50\text{Hz}$ and $A_r=0.5\text{mm}$. The stable point occurs at C where the force is zero. When particle B is at point C, the gap between the particles is about 0.08mm . The length of the largest arrow in the figure corresponds to a force of magnitude $2.6\mu\text{N}$. The bold arrowed-line from B to C shows an approximation to the trajectory followed by B, relative to A, were it free to move. The double arrow at A indicates the direction of oscillation.

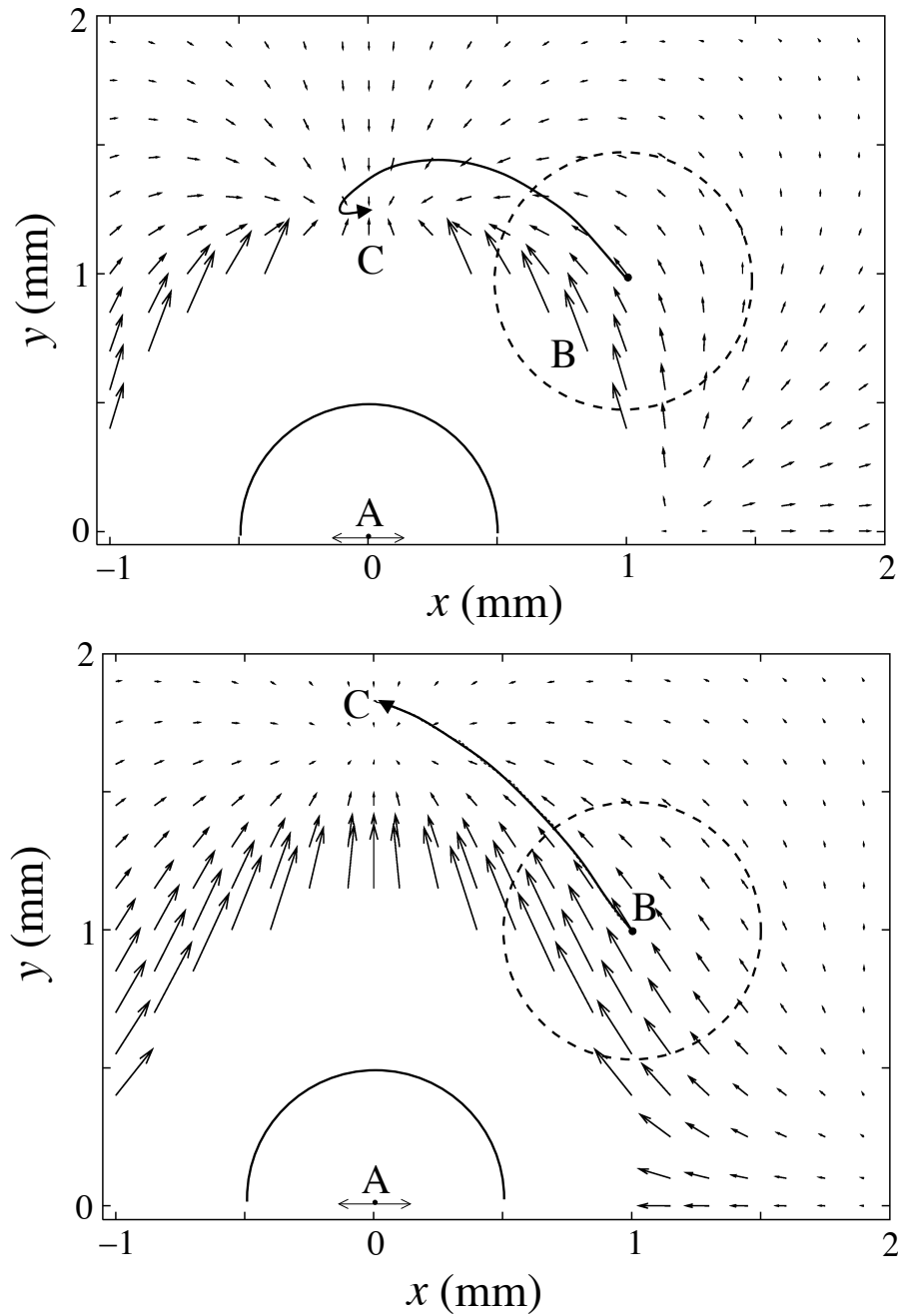


Fig. 5.16: Vector plot of the effective force acting at the centre of particle B placed near particle A, for $\nu=4.5\times10^{-6}\text{m}^2\text{s}^{-1}$, $f=50\text{Hz}$ and $A_r=0.4\text{mm}$ (top) and $\nu=9.4\times10^{-6}\text{m}^2\text{s}^{-1}$, $f=30\text{Hz}$ and $A_r=0.83\text{mm}$ (bottom). The stable point occurs at C where the force is zero. When particle B is at point C, the gap between the particles is about 0.25mm (top) and 1.2mm (bottom). The length of the largest arrow in the top figure corresponds to a force of magnitude μN and in the bottom figure a force of magnitude μN . The bold arrowed-line from B to C shows an approximation to the trajectory followed by B, relative to A, were it free to move. The double arrow at A indicates the direction of oscillation.

which is indicated by point C. Note that we are only showing a portion of the upper half of the space, there is another stable point in the lower half, below particle A. Along that axis (y) perpendicular to the oscillation, there is an attractive or repulsive force depending on separation which leads to the equilibrium spacing at C. Note that the forces along the y -axis have already been discussed in an earlier section. This is also true for different parameters shown in Figs. 5.16 (top) and (bottom). Parallel to the oscillation, along x , in Fig. 5.15, particle B is repelled, and that repulsive force weakens as the viscosity increases, see Fig. 5.16 (top), until it becomes attractive in Fig. 5.16 (bottom).

We remind the reader that in these simulations the particles are locked in position relative to each other, whereas in experiment they are free to move. The bold-arrowed line in Figs. 5.15, 5.16 (top) and (bottom) shows the path followed by B, relative to the position of A, in simulations in which the fluid is oscillated and both particles are free to move. This path does not exactly follow the direction of the calculated forces for two reasons: there is a time-scale over which the streaming flow is set up and the moving particles have inertia. Furthermore, the trajectory for one sphere is shown but it is calculated when two free spheres respond to the flow and align. Nevertheless, the forces give a reasonable indication of the relative motion of the particles and correctly predict the final configuration of a pair in all three sets of parameters.

Any position other than C, leads to a trajectory which re-orientes the pair at right angles to the oscillation, which then sits an equilibrium gap apart. However, the path leading to C changes as the viscosity goes up. Notice that in Figs. 5.15 and 5.16 (top) the forces trace a path which circulates anti-clockwise, shoots off beyond the equilibrium position C due to inertia and then returns whereas in Fig. 5.16 (bottom) it circulates towards point C without overshooting because the Reynolds number is lower. The exact trajectories in each case are shown together in Fig. 5.17. We remind the reader that the trajectories correspond to the real path sphere B traces when both spheres A and B are free to move in response to the oscillating container. The dotted line shows the path of B relative to A for the highest Reynolds number out of the three ($Re=78$). It is evident that sphere B goes back and forth a few times before it settles oscillating at

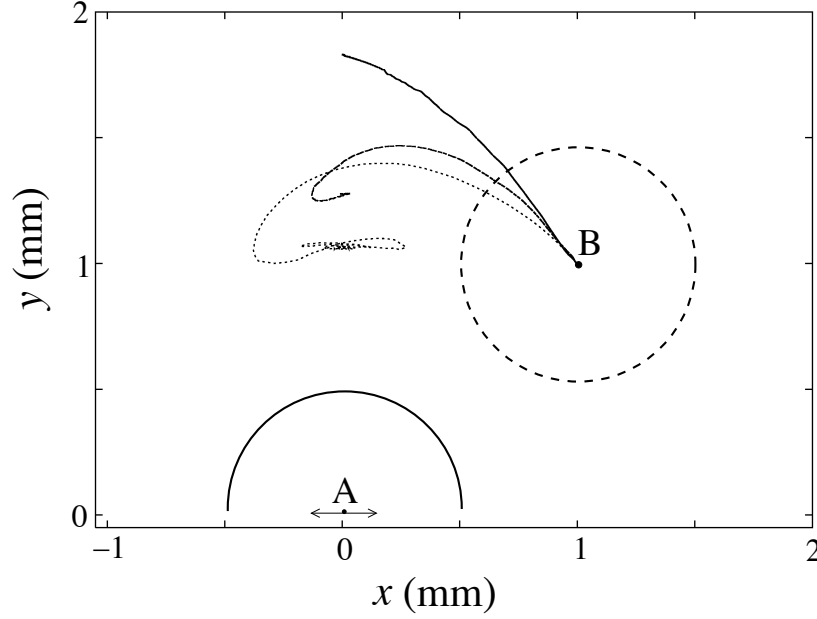


Fig. 5.17: Three different trajectories that sphere B follows near sphere A, when both spheres are free to move in an oscillating fluid at different vibratory parameters and viscosities. Dotted line: $\nu=2.0 \times 10^{-6} \text{m}^2 \text{s}^{-1}$, $f=50 \text{Hz}$ and $A_r=0.5 \text{mm}$. Dashed line: $\nu=4.5 \times 10^{-6} \text{m}^2 \text{s}^{-1}$, $f=50 \text{Hz}$ and $A_r=0.4 \text{mm}$. Solid line: $\nu=9.4 \times 10^{-6} \text{m}^2 \text{s}^{-1}$, $f=30 \text{Hz}$ and $A_r=0.83 \text{mm}$.

equilibrium. As the viscosity goes up and Re goes down, there is less inertia and the path that B traces demonstrates that. Finally, in all plots the result is the same: there is only one equilibrium configuration, for a given set of parameters, and that is a certain distance apart at right angles to the direction of oscillation, denoted by C.

However, we still do not know what the source of this effective force is. Lyubimov *et al.* (2001) predicted this alignment theoretically for two cylinders in inviscid flows and commented that the preferred configuration is always one where the particles expose maximum surface area to the incident flow. It has also been proposed in Voth *et al.* (2002) that the interaction between spheres can be understood by considering the streaming flow generated by a single, isolated sphere. If the two spheres are far apart, each particle tends to follow the flow generated by the other. In order to test this hypothesis, we have run simulations for single isolated oscillating spheres under the same three sets of parameters as in Figs. 5.15, 5.16 (top) and (bottom). In Fig. 5.18 (a)-(c) we show the time-averaged fluid flow for an oscillating sphere corresponding to the parameters of Figs. 5.15, 5.16 (top) and (bottom).

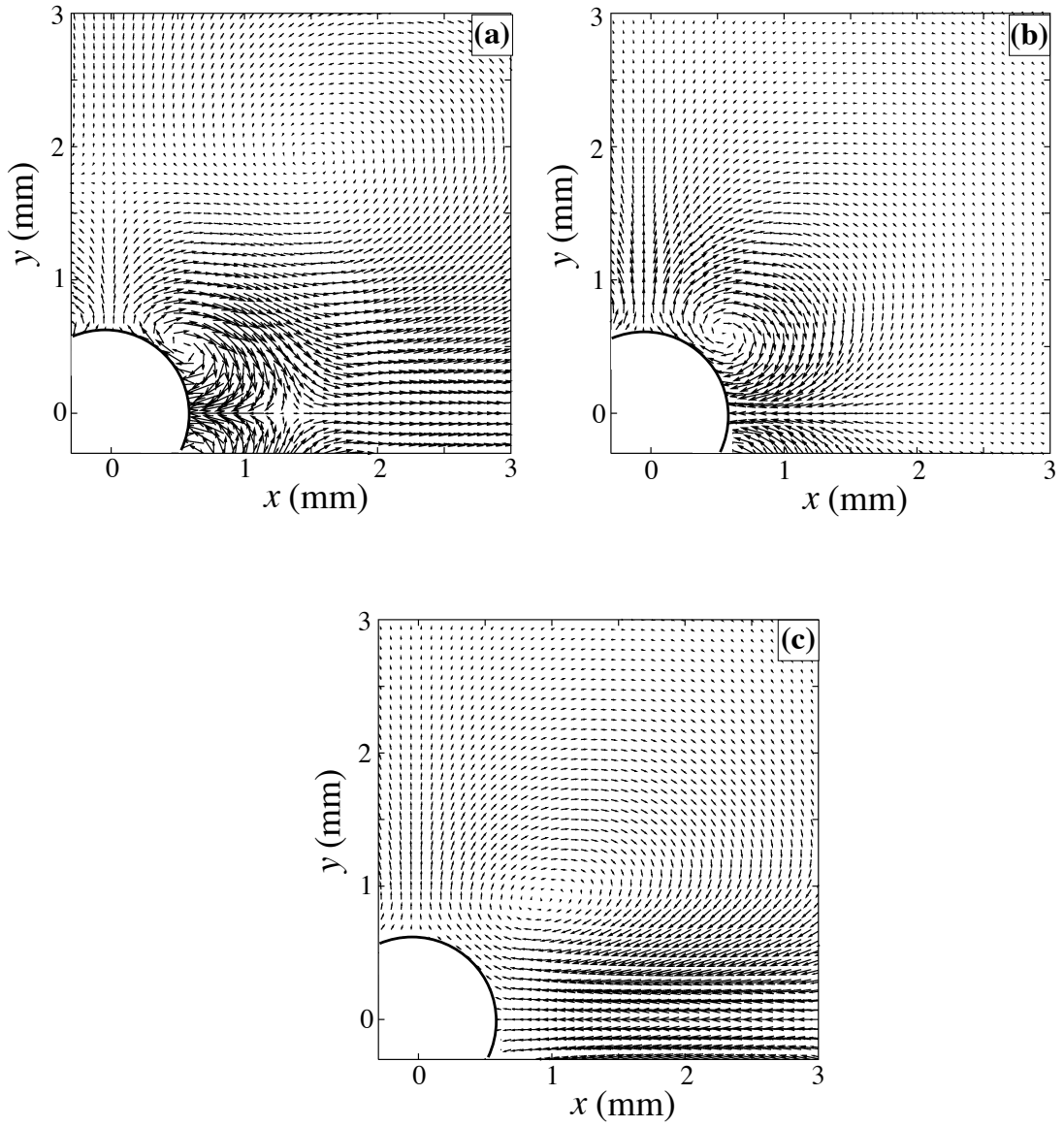


Fig. 5.18: Vector plots taken from simulations, showing part of the time-averaged fluid flow around a single oscillating sphere, for (a) $\nu=2.0\times10^{-6}\text{m}^2\text{s}^{-1}$, $f=50\text{Hz}$ and $A_r=0.5\text{mm}$, (b) $\nu=4.5\times10^{-6}\text{m}^2\text{s}^{-1}$, $f=50\text{Hz}$ and $A_r=0.4\text{mm}$ and (c) $\nu=9.4\times10^{-6}\text{m}^2\text{s}^{-1}$, $f=30\text{Hz}$ and $A_r=0.83\text{mm}$. The sphere is oscillating in the x -direction and the fluid flow in the x - y plane passing through the centre of the sphere is shown. The arrows indicate the local direction of the streaming flow. For reasons of clarity, the magnitude of the arrows is proportional to the product of the local speed and the square of the distance from the origin.

Let us consider Fig. 5.15 and Fig. 5.18(a). For large separations the forces (Fig. 5.15) and the single particle streaming flow (Fig. 5.18(a)) are in the same direction. However, when the two particles are close together this simple picture breaks down. For example, at the point $x=1, y=1$ in Fig. 5.15, the force points upwards and to the left, whereas the flow at the same point in Fig. 5.18(a) points downwards and to the right. The same mismatch can be observed at point (1,1) comparing Fig. 5.16 (top) with Fig. 5.18(b) and Fig. 5.16 (bottom) with Fig. 5.18(c). We therefore conclude that the interaction between two spheres oscillating in a fluid flow maybe somewhat more complex than simple arguments based on single sphere streaming flow would suggest.

5.7 Discussion

In this section the findings of both Chapters 4 and 5 will be discussed, after a brief summary of the key results.

In Chapter 4 we experimentally observed the interaction between two spheres in an oscillating fluid-filled cell. We found that the particles align perpendicular to the direction of oscillation and sit at a well-defined spacing, at equilibrium. Moreover, two scaling regimes for the equilibrium gap were identified at low (LAR) and high amplitudes (HAR).

In the present Chapter, we used simulations to study this interaction between the two spheres. Our main findings are:

We confirmed the experimental scalings where the equilibrium gap scales with δ^2/d in the LAR and with $A_r\delta/d$ in the HAR. The interaction force between the two particles is repulsive at small separations and attractive at long separations as expected from the existence of a gap. In the extremes of the two scaling regimes the interaction force can be predominantly repulsive or attractive. For most parameters both a repulsive at short separations and an attractive component at large separations are present.

The fluid flow for a pair of spheres at equilibrium resembles that of a single object. The outer streaming flow is shared by the pair, keeping it together and making it a very stable entity. We see a change in the average fluid flow between

extremes of the two scaling regimes, the LAR and HAR. The transition is smooth. In the extreme of the LAR outer streaming flow may not be present and the spheres can be predominantly repelling. In the extreme of the HAR there is always outer streaming flow. However, for most parameters in the LAR there is outer streaming flow which grows stronger as the amplitude increases and it shifts towards the HAR.

For an oscillating sphere in a fluid in our geometry there are only two stable positions for another particle to go to, which is at a certain distance apart, perpendicular to the direction of the oscillation. All other positions near the sphere are unstable.

It seems that the inner vorticity which is generated by the no slip boundary condition between the surface of the sphere and the fluid, keeps the spheres a certain distance apart. The inner vorticity is always present in a viscous fluid. As the viscosity goes up the inner streaming expands and requires more space thus pushing the spheres further out, and the gap increases. The outer streaming flow is generated by this inner vorticity and it seems that it is the secondary streaming which is responsible for the attraction. The kinetic energy of the system is lowered because when the spheres form a pair the outer vortex loops are shared by the pair.

Each particle in isolation carries with it four vortex rings, two inner and two outer, and their preferred configuration is one where they interfere so as to have six vortex loops in total and not eight. When these two particles are at an angle their vortex structures interfere; it is favourable to sit in a line and lower the number of vortex rings. The resulting equilibrium flow is the only one which keeps the spheres stable. If the spheres are too close together the inner vortex loops interfere and push the spheres out; if the spheres are further apart the outer vortex loops interfere and the spheres are brought together. If the spheres are really far enough so that there is no interference then each sphere has the vortex structure of an isolated sphere; in this case the spheres are not interacting.

For each oscillating sphere, in our geometry, there are only two equilibrium positions that another particle would go to. In fact, if we imagine the flow in three dimensions, we see that for each oscillating isolated sphere there is a ring of

stable positions on either side of the sphere, similar to the ring of stagnation points where the inner vortex rings end. This is very interesting because it implies that these steady streaming flows would form layers of spheres in three dimensions.

The flow we saw for the extreme of the HAR may be related to separation of flow. It is known that separation of flow occurs above a Reynolds number in steady flows and above a certain amplitude for an oscillating single sphere. Chang and Maxey (1994) and Riley (1966) have reported that secondary steady streaming may occur due to separation of flow above a certain Re , which corresponds to a low-frequency, high amplitude case. From our simulations we know that there is secondary streaming in lower amplitudes where separation of flow does not seem to occur and which would be in our low amplitude scaling regime, LAR. However it may be the case that towards the highest of amplitudes in the HAR, separation of flow also occurs.

Finally we shall end this chapter reminding the reader that at this point the most important finding is that a bound pair of spheres behaves as a single object as far as the outer streaming flow is concerned. If this is true it implies, according to Figs. 5.15 5.16 (top) and (bottom), that for the pair too there are two stable points where a third and fourth sphere would sit at, if they were added into the system. Multiple-sphere systems are the subject of the following chapter.

Chapter 6

Multiple-particle systems

In this chapter, we build on our earlier work by considering the interactions between many particles in a fluid subjected to horizontal vibration. Thus, we shall finally reach our original goal which was to understand in detail the mechanisms behind the interactions of multiple-particle systems which are responsible for the chain structures observed by Wunenburger *et al.* (2002) and the clusters reported by Voth *et al.* (2002).

So far, we have seen experimentally and from simulations how two spheres align perpendicular to the direction of vibration. We have quantified the size of the equilibrium gap between them, and also identified two regimes of behaviour. Through force measurements it was shown that for a single isolated oscillating sphere in the two-dimensional cell there are two equilibrium positions, (see Fig. 5.15 and caption). Furthermore, we have explained that when the system goes from a single sphere to a bound pair, the outer streaming flow for the pair resembles that of a single sphere.

What happens if a third or fourth particle is added and so on? We might expect that chains of particles will form perpendicular to the axis of vibration, as was found by Wunenburger *et al.* (2002).

The outline of the chapter is as follows. First we describe the experimental arrangement and our experimental observations, on the formation and evolution of chains. We then briefly explain the simulation method used to model the particular experiments, (though full details are found in Chapter 2), and we present computational results on the formation and evolution of chains. A direct

comparison between experiment and simulation will be discussed. We shall then use simulations to study in detail all the stages of the chain-forming mechanism. In the end there will be a discussion on pattern formation.

6.1 Multiple-particle experiments

6.1.1 Experimental arrangement

We conducted our experiments using spheres fully immersed in a liquid contained in a small cell which was subjected to horizontal vibration. Specifically, the cell was constructed in the following way. A rectangular hole was cut into a 3mm thick rubber sheet which was sandwiched between two glass plates, supported by an aluminium alloy frame, as shown in Fig. 6.1 (a). The dimensions of the resulting liquid-tight region were 39.5 mm long (x -direction, horizontal), 11.5 mm wide (y -direction, horizontal) and 3 mm deep (z -direction, vertical). In Fig. 6.1 (a) and (b) a photo and a schematic diagram of the cell are shown respectively. The liquid and the spheres were placed in the cell before it was sealed.

Note that the region available to the fluid and the spheres is smaller than the one used for the two particle experiments in Chapter 4. The reason is that as more spheres are added into the system, the simulation becomes computationally more intensive, and in order to be able to directly compare between experiments and simulations, we save on computational power by using a smaller container in both experiments and simulations.

The cell was mounted between two long-throw loudspeakers so that the plane of the glass sheets (x - y plane) was accurately horizontal during vibratory motion such that only one-dimensional motion in the x -direction occurred. We remind the reader that the sinusoidal motion may be characterised by the frequency, f , and by the dimensionless acceleration of the cell, $\Gamma = A\omega^2/g$, which was determined using capacitive acceleration sensors. A is the amplitude of the vibration, $\omega = 2\pi f$ is the angular frequency and g is the gravitational acceleration.

We used a solution of glycerol and water with kinematic viscosity $\nu = 2.0 \times 10^{-6} \text{m}^2 \text{s}^{-1}$ at 22°C. The laboratory and cell were kept at this temperature to avoid changes in the viscosity. The fluid density was $1,060 \text{ kg m}^{-3}$. The fluid

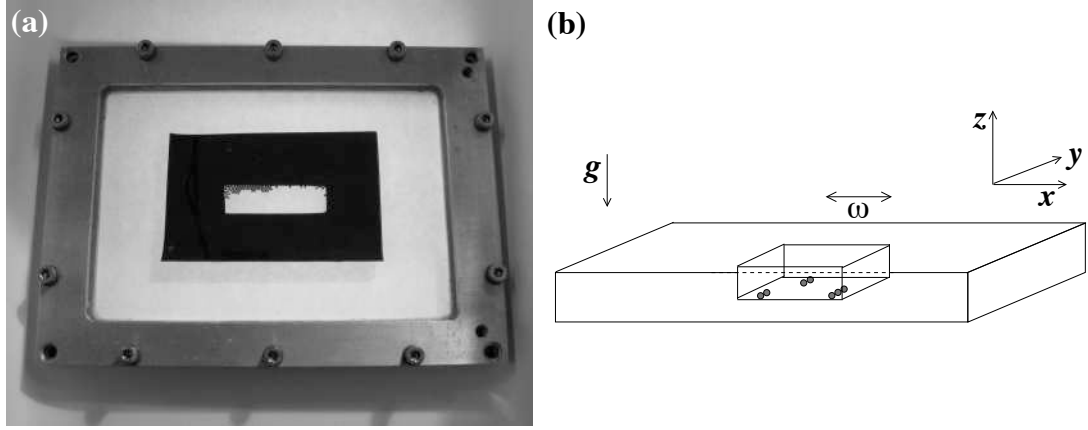


Fig. 6.1: (a) A top-view picture of the cell used in our experiments. The black rectangle is the rubber gasket. The region inside is where the fluid and the spheres are. (b) A schematic diagram of the same cell. The three axes x , y , z are indicated, as well as the direction of the gravitational acceleration g and the axis of oscillation ω .

was pumped prior to the experiment so as to remove any dissolved air. The cell was then sealed so that no air was trapped in it. The particles used were non-magnetic, stainless-steel spheres, 1mm in diameter and of density $7,950 \text{ kg m}^{-3}$. A high-speed camera (up to 1,000 f.p.s.) was mounted directly above the cell so that the motion of the spheres could be displayed and recorded.

All the experiments reported here were carried out at $f=50\text{Hz}$ and with $\Gamma=6.5$. The corresponding relative amplitude of the spheres, A_r , was measured to be $0.5\text{mm} \pm 0.05\text{mm}$, whereas the driving amplitude was $A=0.65\text{mm}$. The viscosity, frequency, Γ and the number of spheres are all fixed. The goal is to focus on one set of parameters and try to understand the chain formation in detail. However, we have checked that chains of spheres do indeed form perpendicular to the axis of vibration over a range of $f=10\text{-}60\text{Hz}$, $\Gamma=1.5\text{-}7$ and $\nu=1.0 \times 10^{-6} - 9.4 \times 10^{-6} \text{ m}^2\text{s}^{-1}$.

6.1.2 Experimental procedure

Sixty-four spheres were initially placed in the cell which was shaken manually, before being mounted onto the vibratory apparatus. The subsequent motion of the spheres was recorded on the high-speed camera and replayed at a low frame-per-second rate so that the process could be observed in detail.

As soon as the vibration is switched on the particles rapidly form chains within

the first few seconds. The amplitude and the frequency are varied and we observe that chains indeed always form over the usual range. As with the two-particle experiments, described in Chapter 4, the Γ range corresponds to the fact that below a certain amplitude the interactions are too weak and above a maximum amplitude the fluctuations of each particle in a chain are huge.

In Figs. 6.2 and 6.3 we show ten characteristic snapshots from the experiment, along with their times, over 21s. The formation of chains and the general behaviour is evident from the images. However, in order to make it easier for the reader, we coloured on the image three different spheres whose exact trajectories can easily be traced. Their distinct paths capture the main features of the system and will be discussed in detail. Let us consider the general trends first and then focus on each of the coloured spheres.

As soon as the vibration is switched on, nearby particles align in pairs, the line joining their centres tending to orient perpendicular to the direction of the oscillation. A free particle moves so that it joins the nearest pair to form a short chain. Similarly, a free pair joins another nearby pair also forming a short chain. There is also a tendency for particles and chains to attach to the long sides of the cell. Short chains then evolve to form longer ones by attaching at the ends of their nearest chain. Long chains form which span the cell between the two long sides. The stages described so far have occurred almost within the first 2s of oscillation, $t=2.12$ s Fig. 6.3. Everything which follows happens at a much slower rate as the system evolves towards its final configuration in which there are no free particles or free chains, as they are all attached to at least one of the side walls.

Now let us consider the coloured particles: the blue, the green and the red. The initial positions of the particles in the cell are: near a wall (blue), left-middle of the cell (green), right-middle of the cell (red).

The blue sphere attaches itself to the wall on one side, within 0.14s (Fig. 6.2), and then attracts the nearest neighbour on the other side to form a pair by 0.21s. The pair oscillates attached to the wall for the next few snapshots. By $t=0.44$ s it looks like another sphere is attracted to the free end of the pair. Indeed that particle makes its way (seen at $t=0.61$ s) and attaches itself to the

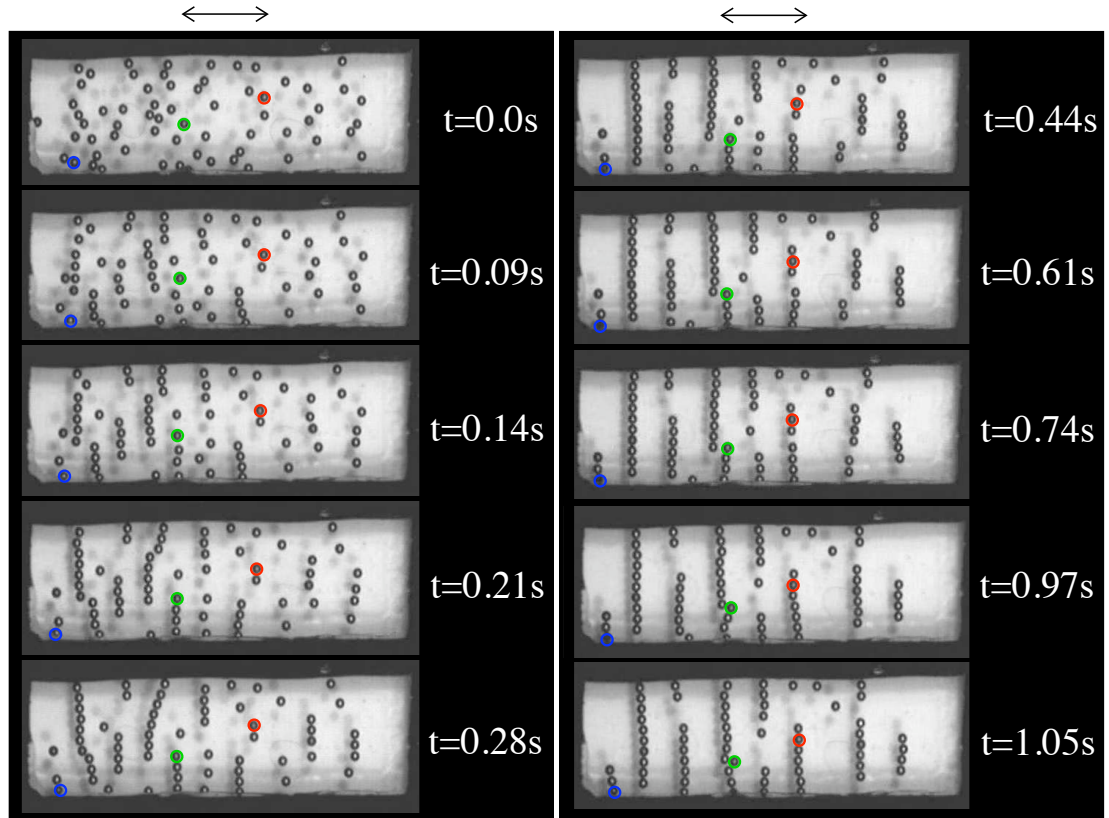


Fig. 6.2: The first ten of a series of twenty snapshots, taken from experiment, showing the the first second of evolution of sixty-four spheres under horizontal vibration, from an initial dispersed configuration at $t=0.0$ evolving towards an ordered state. Three different particles have been coloured so that their trajectories can easily be traced; they are characteristic of the system. By 0.14s: the nearest spheres have interacted with each other; pairs have started to form, aligning perpendicular to the direction of oscillation. Between 0.14s and 0.44s: short chains form; there is also a tendency for particles and chains to attach to the side walls. Between 0.44s and 1.05s: short chains evolve to form longer ones by attaching at the ends of the nearest chain; or they attach to the side walls.

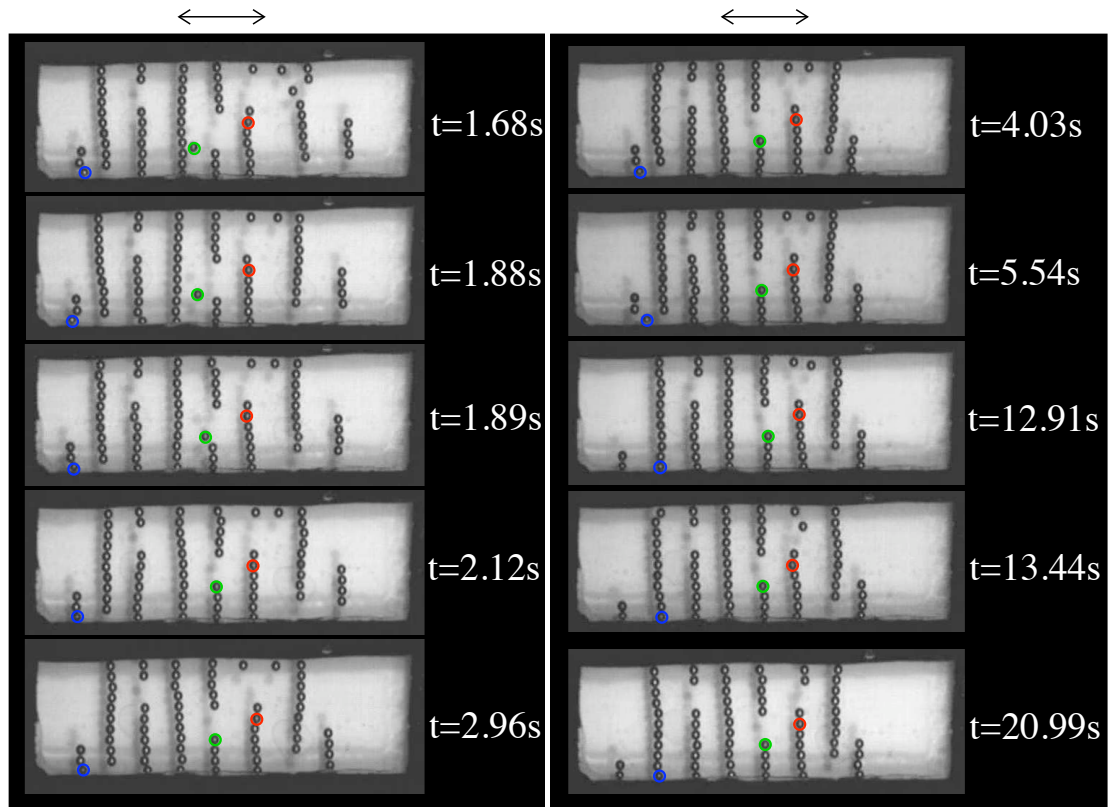


Fig. 6.3: The second half of a series of twenty snapshots taken from experiment, showing the evolution of sixty-four spheres under horizontal vibration, which have already formed chains, from $t=1.68\text{s}$ to an ordered state after about 20.0s , under horizontal vibration. The same three particles as in Fig. 6.2 have been coloured so that their trajectories can easily be traced; they are characteristic of the system. After 2.0s , most particles are either part of a chain or are attached to the wall; there are no free particles. Thereafter the arrangement appears to be more-or-less stable.

pair, to form a three-particle chain, visible at $t=0.74\text{s}$. The short chain oscillates attached to the wall via the blue sphere for almost another second. However, as the surrounding configuration has also evolved, at $t=1.68\text{s}$ (Fig. 6.3) it seems that the blue sphere is attracted to the incomplete chain right next to it. The blue sphere wiggles back and forth for almost 4s from $t=1.68\text{s}$ - 5.54s (which is a long time compared to the time scale over which chains initially formed) until it finally joins the neighbouring chain, shown at $t=12.91\text{s}$. The blue sphere is now part of a full chain (a chain that spans the width of the cell), which remains stable until the end of the experiment $t=20.99\text{s}$.

The green sphere is initially positioned towards the left-middle of the cell. As soon as the vibration is switched on, it aligns with its nearest-neighbouring spheres as can be seen at $t=0.14\text{s}$. By 0.21s they have formed a four-particle chain which is also attached to the wall on one side. The green sphere is the free end of that chain. At 0.44s it looks like there is a longer chain attached to the opposite wall, and on the left, whose free end is attracted to the green particle. At $t=0.97\text{s}$, the two opposite chains have joined at their free ends. However, because there are more spheres than can be accommodated by the width of the cell, the resulting chain is “overfull” by one sphere, as can be seen at $t=0.97\text{s}$ and $t=1.05\text{s}$. The overfull chain is unstable because it cannot align properly perpendicular to the oscillation, due to lack of space. Consequently, one particle has to leave. The green particle leaves the chain, as can be seen at $t=1.68\text{s}$ and $t=1.88\text{s}$ and attaches itself to the nearest free-end of a chain to form a four-particle chain, seen at $t=2.12\text{s}$. The green sphere remains on this chain until the end of the experiment.

Let us now study the red sphere, which is initially positioned towards the right-middle of the cell far from walls. By 0.14s , the red sphere forms a pair with another single sphere in its vicinity. The pair aligns perpendicular to the axis of oscillation and remains so, vibrating in the cell as a single object for the next 30ms. At $t=0.44\text{s}$ it seems that the pair is attracting another sphere which then joins up to form a three-particle chain at $t=0.61\text{s}$, the red particle in the middle. The short chain then moves as a whole towards the free end of another four-particle chain, which is attached to the wall on one side, seen at $t=0.61\text{s}$ and

$t=0.74$ s. At $t=0.97$ s the short chain with the red particle has joined the free end of that nearest chain and it will remain there until the end of the experiment.

The experiment has been repeated several times under the same vibratory conditions but with different initial positions of the spheres. Each time the exact positions of the spheres in the final configuration are different. However, the time scale for the evolution is always comparable, and the system goes through the same stages of evolution, outlined in the previous paragraphs and shown in Figs. 6.2 and 6.3, always resulting in a more-or-less stable chain configuration.

6.1.3 Discussion on the evolution of chains from experiments

We have observed the general behaviour over many runs and the exact trajectories of three characteristic particles, over 21s of vibration, in which chains of spheres form from an initially random configuration. We are therefore in a position to make the following statements:

1. It takes 1s-2s for most spheres to be parts of chains or to be attached to one of the side walls. It is highly unlikely that there are single free particles oscillating in the cell for $t > 2$ s.
2. Pairs and free-ended chains act like single objects, in the sense that they oscillate and migrate intact, and attract other single spheres or free ends of pairs/chains onto their free ends.
3. Any entity, single sphere, pair or chain, moving freely in the bulk of the cell is stable as an entity but sooner or later it attaches to another free end of a chain or a side wall to increase its stability. In the run presented here in Figs. 6.2 and 6.3 this took 3s.
4. The most stable entity is a ‘full chain’, which we define to be one, which is aligned perpendicular to the direction of vibration and has the correct number of particles to just span the cell. This chain fulfils the two major tendencies of the spheres: to be attached to the walls and to be attached

to other spheres. Such a chain has never been seen to break under the conditions studied here.

5. Sometimes chains merge giving an excess of particles compared to a full chain. The overfull chain is unstable. The extra particle forms a defect, which may move up and down the chain, until a particle leaves that chain. The green sphere was an example shown leaving the chain in Fig.6.3 between $t=1.68\text{s}$ - 1.89s .
6. Because the system tries to produce full chains, the free end of an incomplete chain attracts free particles or the free ends of other incomplete chains in its proximity. Moreover two incomplete chains will align attached to opposite walls; this looks like one chain with some particles missing. An example is shown in Fig. 6.3 from $t=2.12\text{s}$, where the chain with the green sphere and another five-particle chain on the opposite wall are aligned.
7. Within the first few seconds, here 3s, an initial equilibrium is reached, where there are no freely-moving chains or particles. From then on, however, the chains still evolve and there may be the need for a sphere/chain to move from a seemingly stable position to a more favourable stable one. For example the blue particle unexpectedly left a chain to join another one, shown in Fig. 6.3 between $t=4.03\text{s}$ - 12.91s . It is a different stage of evolution where things take place much more slowly. Another situation that could happen is for example the green sphere, which although in a stable position as part of a chain (Fig. 6.2 from $t=0.21\text{s}$), ended up in an overfull unstable chain (Fig. 6.2 at $t=1.05\text{s}$), which it then had to leave. On the other hand, the red sphere remained at the same initial equilibrium position it reached at $t=0.97\text{s}$, Fig. 6.2.
8. Beyond the 21s shown here, there may be an occasional random particle that bounces off an end wall or jumps from one chain to another. That apart, the configuration remains stable over the duration of our experiments, typically a time of the order of minutes.

The particles in Figs. 6.2 and 6.3 which form a chain appear to be in contact. However, from Chapters 4 and 5 and in Klotz *et al.* (2007) it is known that

two particles forming a pair have a well-defined gap between them. We note that under the vibratory conditions considered here, the gap is quite small, of order 0.08mm, as expected.

We have not conducted a study over a large parameter space. However, we did test to see what happens when the vibratory conditions and the fluid viscosities change. At fixed viscosity $\nu=2.0 \times 10^{-6}\text{m}^2\text{s}^{-1}$, when Γ is increased the initial alignment and formation of chains takes place more rapidly. Moreover, it is more likely that the system rearranges from one quasi-equilibrium configuration to another, see previous paragraph, point 7. At higher viscosities, $\nu=4.5 \times 10^{-6}\text{m}^2\text{s}^{-1}$ and $\nu=9.4 \times 10^{-6}\text{m}^2\text{s}^{-1}$, the system slows down and is less turbulent. The gaps between the spheres of pairs or chains are larger. Because the gaps between adjacent spheres in a chain are larger it is easy for a particle to be attracted to the middle of a chain as well as the free end. We also notice that chains are likely to interleave rather than join end on.

If the number of particles is increased in the same container, and because the system always tries to produce full chains, we can imagine that the half-full chains of the final snapshot in Fig. 6.3 would fill up, the configuration looking very similar. If we keep adding particles, we expect that overfull chains form, making the system less stable. More and more overfull chains would form if the number of particles still increases. Note that in overfull chains spheres are very likely to jump from chain to chain in an attempt to stabilise somewhere. If this is not possible they keep moving around. If the number of spheres is very large then the chain configuration does not stabilise.

We have not quantified whether it is more stable to be part of a chain or part of pair although we suspect the bigger the entity the more stable. For example why is it better for the blue particle to leave the short chain it is already part of, and the wall to which it is attached, and go to the neighbouring chain in order to fill it up completely, to make a full chain? Perhaps the greater stability of a long chain leads to this transition.

In the final configuration of Fig. 6.3 it seems like there is an equal spacing between the chains. Such an arrangement can result from an attraction and a repulsion between chains, a repulsion alone, or it could be related to the size of

the container. Irrespective of the details, this interaction between chains is much weaker and the time-scales are longer. In order to measure the effects of such weak interactions, we needed to ensure the horizontality of our apparatus more accurately. The slightest bias, in the container, or the vibration would result in the spheres rolling down the gravitational potential. The horizontality was verified using a Spectra-Physics He-Ne 95mW Class II laser beam which was set up to shine onto the cell and the reflection was observed. (For more details we refer the reader to Wright 2009, p.188). However, we observed a tendency of the spheres and chains to locate themselves towards the middle of the container further from the end walls, at long time-scales. For this reason, we did not include the interaction between chains in our experimental study. We rather decided to investigate this problem through simulations, as we shall see in the next section, where issues of horizontality of the container and vertical oscillation do not arise.

6.2 Multiple-particle simulations

At the start of the chapter, we mentioned that the reason why the multiple-particle experiments were performed in a smaller region was because it would then be possible to simulate the experiments as closely as possible. Using the same computational model as before, described in detail in Chapter 2, it would be extremely computationally demanding to simulate sixty-four spheres in the whole cell, with the same resolution for the fluid grid. We also describe simulations in a different (square) box with fewer particles which were performed in order to study certain details of the chain formation.

6.2.1 Computational Details

The simulations were carried out using a time step $\Delta t = 10^{-6}$ s and a grid spacing $\Delta x = 7.5 \times 10^{-5}$ m. In some of the simulations, we used a rectangular slab with dimensions $39.5\text{mm} \times 11.5\text{mm} \times 3\text{mm}$, as in experiments. In the rest we used a square box with dimensions $30\text{mm} \times 30\text{mm} \times 3\text{mm}$ so as to study interactions between particles or chains which are far from walls.

Two types of simulation have been performed: In one, the system was chosen

to model the experimental arrangement as closely as possible. The box and the fluid were oscillated and the spheres were free to respond to the oscillation. The driving amplitude $A=g\Gamma/\omega^2$ was tuned so that the relative amplitude of the spheres with respect to the fluid was the same as in the experiment, $A_r=0.5$ mm. Here we used the rectangular slab with dimensions $39.5\text{mm}\times 11.5\text{mm}\times 3\text{mm}$, as in experiments.

In the other type of simulation, the spheres were fixed at some constant relative position and were oscillated sinusoidally with relative amplitude $A_r=0.5\text{mm}$ with respect to the fluid. Here, the fluid flow was generated by the motion of the spheres. Once a steady state had been reached (that is, the fluid velocities oscillated periodically at the driving frequency) the time-averaged forces on the spheres and the corresponding fluid flows could be determined. In some of these simulations we used the rectangular slab and in some a square one with dimensions $30\text{mm}\times 30\text{mm}\times 3\text{mm}$, when we wanted to study interactions and flows of spheres away from walls.

In all the simulations the vibratory conditions and fluid viscosity are fixed to the same values as the experiments described before, namely $f=50\text{Hz}$, $A_r=0.5\text{mm}$ and the viscosity is $\nu=2.0\times 10^{-6}\text{m}^2\text{s}^{-1}$.

6.2.2 Computational results and comparison with experiment

In Figs. 6.4 and 6.5 we show a series of twenty-two snapshots taken from simulation, where the formation and evolution of chains is shown from an initially dispersed configuration to an ordered state at 13.44s. The images taken in the first 3s, match exactly the times that images were shown from experiments in Figs. 6.2 and 6.3. For $t>2.96\text{s}$, the simulation images were picked so as to illustrate best the evolution of the specific system. Even though the initial positions of the particles were different from those in the experiments, similar chain patterns formed over the same time scales. Simulations with different initial positions of particles led to different final chain configurations but all went through similar stages of evolution.

We observed the same behaviour as in the experiments. As soon as the vibra-

tion is switched on, pairs and short chains rapidly form; they are also attracted to the side walls. Within 1.05s (Fig. 6.4) of oscillation, there are no single spheres in the bulk of the cell; they are all either attached to the wall or to other spheres or both. Pairs and short chains migrate intact attracting other particles along their paths to attach onto their free ends; notice for example the free pair and the free short chain between $t=1.68\text{s}$ - 2.96s (Fig. 6.5). By 3s there are no isolated spheres, pairs or chains, as they are all attached to at least one of the side walls. As observed in experiments, by 3s, an initial equilibrium state has been reached. From now on everything happens at a much slower rate. There is an overfull chain on the far left, at $t=2.96\text{s}$. The chain loses the extra particle, which then attaches itself to the nearest wall and remains there until the end of the simulation. Two incomplete chains attached to opposite walls ($t=4.30\text{s}$. on the right) merge to form an overfull chain, which is now unstable, seen at $t=6.54\text{s}$. Moreover a three-sphere chain on the far right keeps colliding with the right wall as can be seen at $t=6.54\text{s}$. This constant collision is unstable and so the particles one by one gain enough momentum from the collision and bounce off the wall breaking through the chain to the left between $t=6.54\text{s}$.- 9.88s . The configuration is stable by 10s, and remains as such until the end of the simulation which is at $t=40\text{s}$.

The similarities between experiment and simulation are evident from Figs. 6.2,6.3 and Figs. 6.4, 6.5. The same principles formulated for the experiments are also observed in simulations. We are, therefore, reasonably confident that we can use the same computational model to study the system in more depth.

6.3 Details of chain formation

In order to understand the details involved in the formation of chains, we have investigated each step of their development separately, so as to build up a picture which explains the evolution towards a stable configuration. Here, we shall study the formation of short chains and how they interact to produce a long one; the evolution of full chains which span the cell, and the interaction between neighbouring chains.

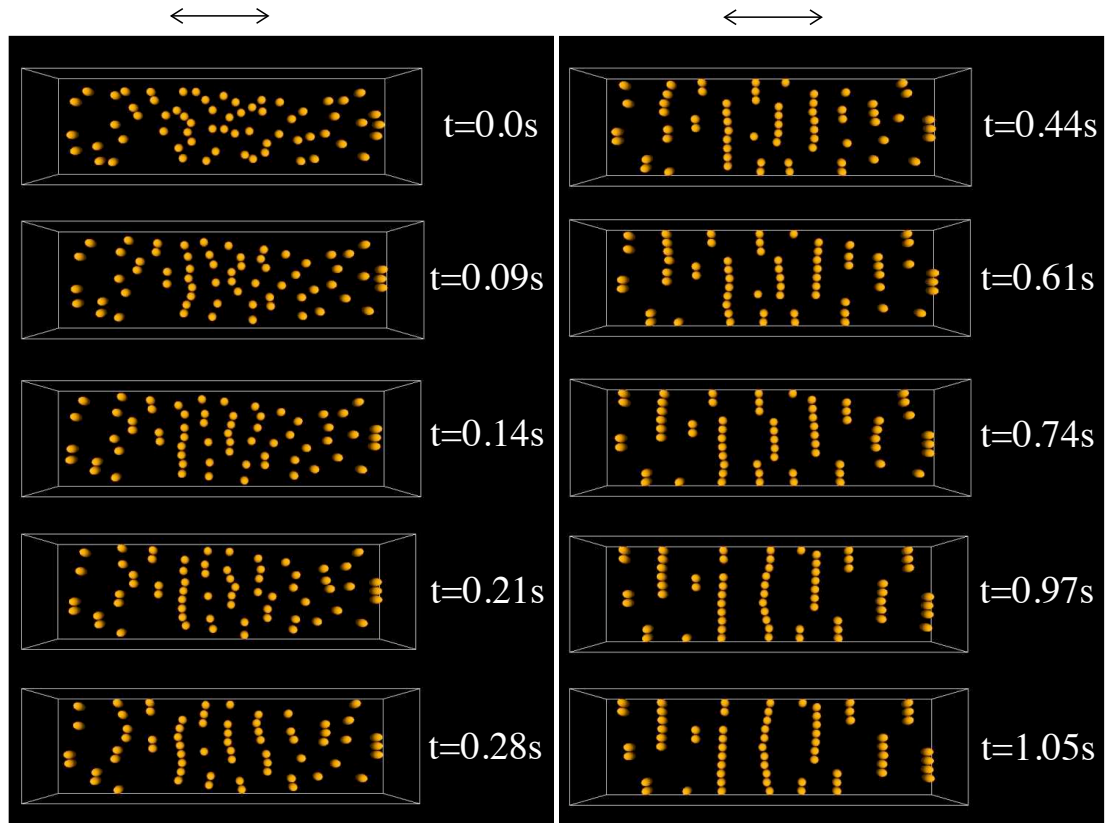


Fig. 6.4: The first ten of a series of twenty-two snapshots taken from a simulation of the experimental system (Fig. 6.2) showing the initial steps of the formation of chains from $t=0.0\text{s}$ to $t=1.05\text{s}$. The particles go through the same stages of evolution as in the experiment, even though the initial positions and the final stable configuration differ. The time scales for the evolution are also comparable.

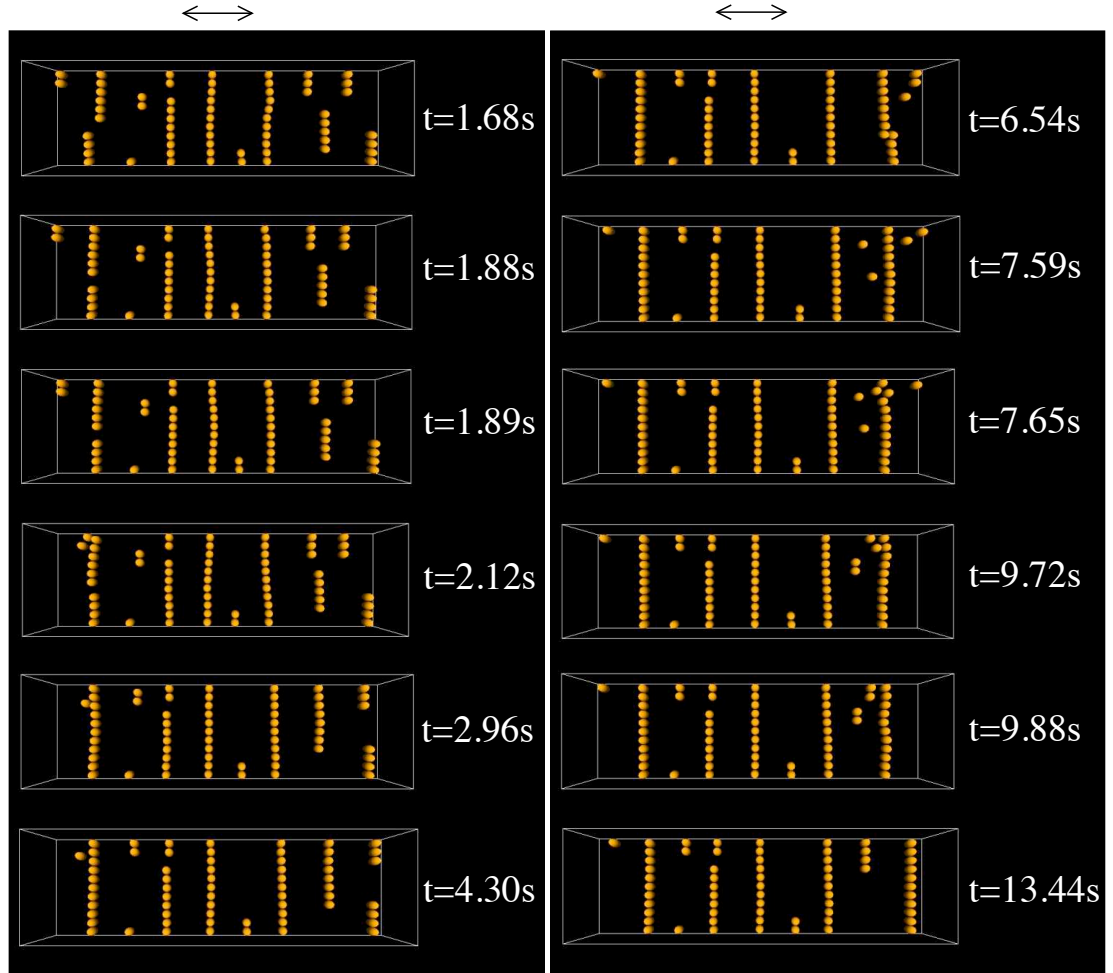


Fig. 6.5: The second part of a series of twenty-two snapshots taken from a simulation of the experimental system (Fig. 6.3) showing the evolution of chains from $t=1.68\text{s}$ to $t=13.44\text{s}$. The particles go through the same stages of evolution as in experiment, even though the initial positions and the final stable configuration differ. The time scales for the evolution are also comparable.

6.3.1 Formation of a short chain

The main concepts have already been formulated in previous chapters, 4 and 5. We have shown that for a single oscillating sphere, there are two equilibrium points in the vicinity of the sphere, which lie on an axis perpendicular to the axis of oscillation, see Fig. 5.15. When two spheres are present, under vibration, they form a pair, aligned in this way. The outer streaming flow from a pair resembles that of a single sphere. (There are two outer vortex rings for a single sphere and there are two outer vortex rings for a pair, *not four*). We can therefore make the supposition that for a pair too there are two equilibrium points, on an axis perpendicular to the axis of oscillation. It would then be straightforward to assume that a third particle would attach itself to the pair on one of the two equilibrium points, thus forming a short chain. Furthermore, we would expect pairs of spheres to interact with other pairs in an analogous fashion to the way single spheres interact. Consequently, pairs would join together to form short chains. Similarly a pair and a single sphere would interact in the same way. Through simulations we can investigate in detail whether this is true.

First we consider the fluid flow around a short chain. We ran simulations in which a short chain is oscillated and the fluid flows are generated by that motion. The spheres in the chain are forced to oscillate in phase; they are not free to move in any other way. After a steady state has been reached, we take an average of the fluid flow over one cycle of oscillation. Fig. 6.6 (a) is a vector plot of the local speed of the fluid, showing the streaming flow for the four-sphere chain in the x - y plane through the centre of the spheres. Only part of the flow is shown, near the chain. In Fig. 6.6 (b) a schematic diagram of the flow is shown. Notice that as for the pair of spheres, the short chain also has a similar outer streaming flow to that of a single object. Remember there are two outer vortex loops for a single oscillating sphere. Here it can be seen that for four oscillating spheres at the equilibrium configuration of a short chain, there are also only two outer vortex loops, one on either side of the chain. Each vortex loop is elongated in the direction parallel to the chain and terminates on the bottom surface of the cell slightly beyond the ends of the chain. In this way the chain is held together, as a single object attracting more particles at the free ends.

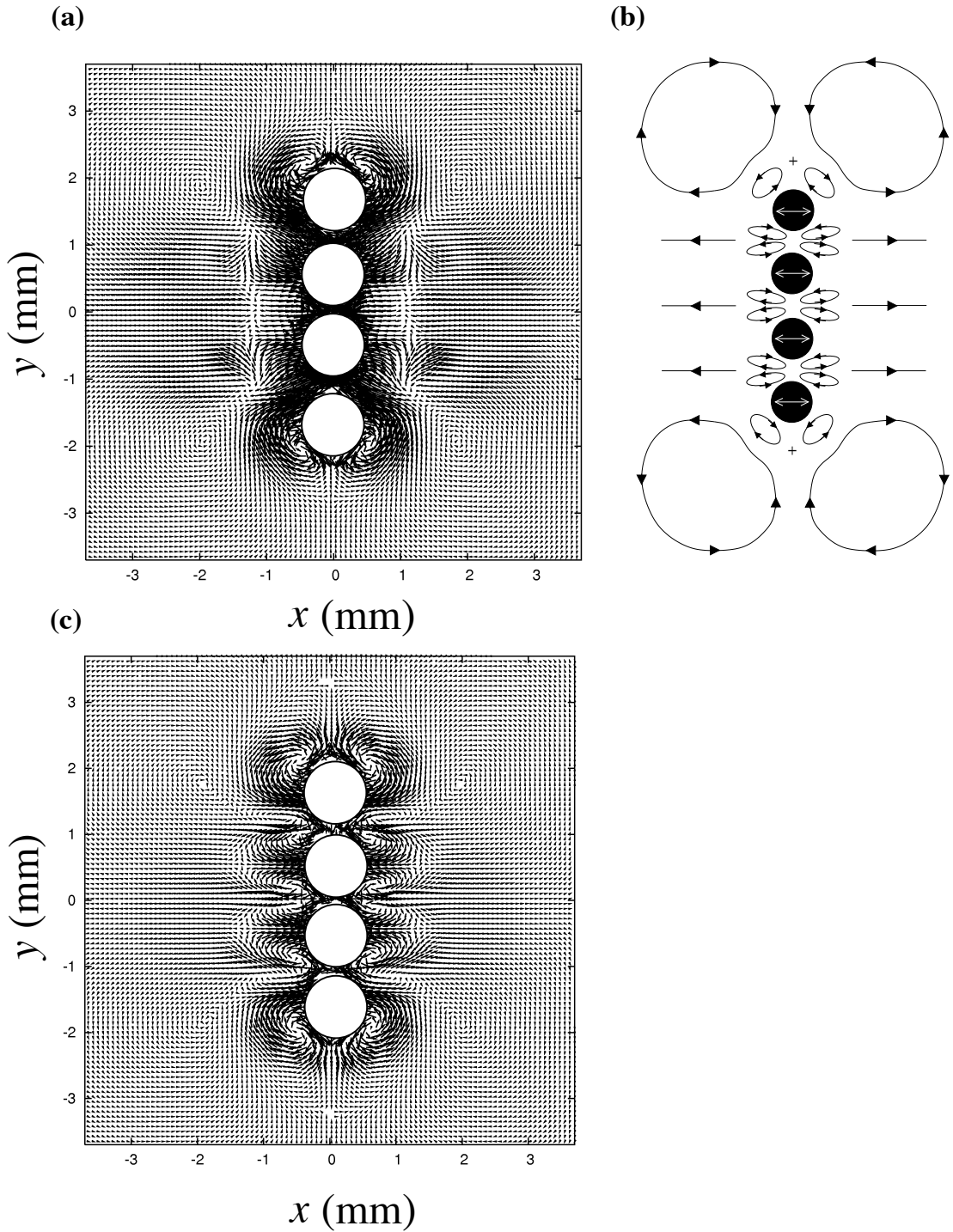


Fig. 6.6: The fluid flow around a short four-particle chain. In (a) and (c) we show, vector plots taken from simulation, showing part of the time-averaged fluid flow for the short chain. The spheres are oscillating in the x -direction. The fluid flow in the x - y plane passing through the centre of the spheres is plotted in (a) and the fluid flow in the x - y plane passing *below* the centre of the spheres is plotted in (c). A schematic diagram of this flow is drawn in (b). Crosses indicate stagnation points. The double arrowed line on each sphere indicates the direction of oscillation, x .

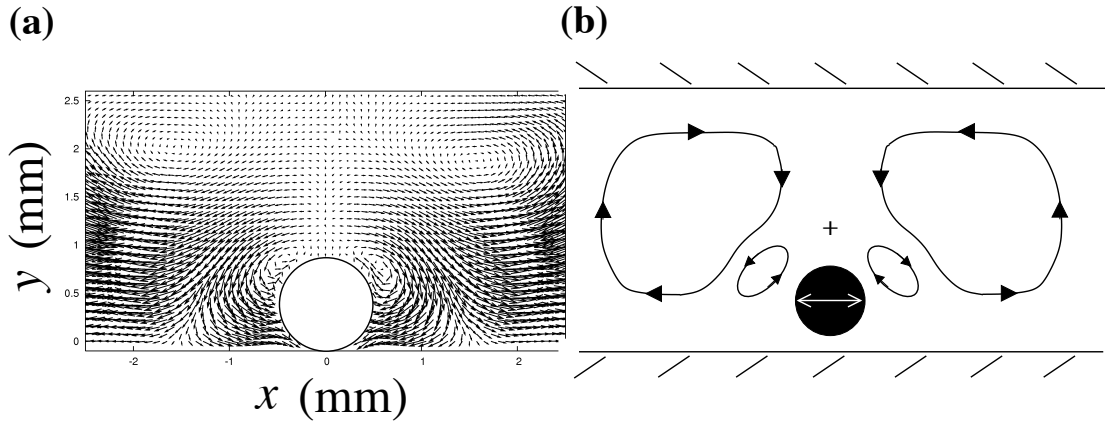


Fig. 6.7: (a) A vector plot taken from simulations, showing part of the time-averaged fluid flow around one of the spheres of a four particle chain. The spheres are oscillating in the x -direction and the fluid flow in the x - z plane passing through the centre of one of the spheres is shown. For reasons of clarity, the magnitude of the arrows is proportional to the product of the local speed and the square of the distance from the mean position of the centre of the sphere. A schematic diagram of the flow is shown in (b). The cross indicates a stagnation point. The double arrowed line on the sphere indicates the direction of oscillation.

Let us consider the inner vorticity. In Fig. 6.6 (c) we show a vector plot from simulation, for the fluid flow in the x - y plane passing *below* the centre of the spheres, at $z=0.375\text{mm}$. (The centre of the spheres is at $z=0.6\text{mm}$.) The inner vortex loops for each sphere are more clear here than in (a).

A vector plot of the flow in the x - z plane through the centre of one of the spheres of the chain is shown in Fig. 6.7 (a). A schematic diagram of the flow is shown in Fig. 6.7 (b). The structure in this plane is the same as that of a single particle.

We have repeated the simulation with more spheres in the chain. The strength of the outer vortex loops increases with the number of particles in a chain because it is driven by more inner vortex loops. The outer streaming flow pattern has the same structure as that of a single pair.

As a further elaboration of our picture of chain formation we have run simulations in which four-particle chains are shaken at a fixed orientation relative to each other in order to measure the forces between them. An example is shown in Fig. 6.8. The arrows indicate the time-averaged force on each particle in the chain due to the flows around the chains. The overall force leads to an attraction between the nearest ends of the chains. Note that the forces are not pair-wise

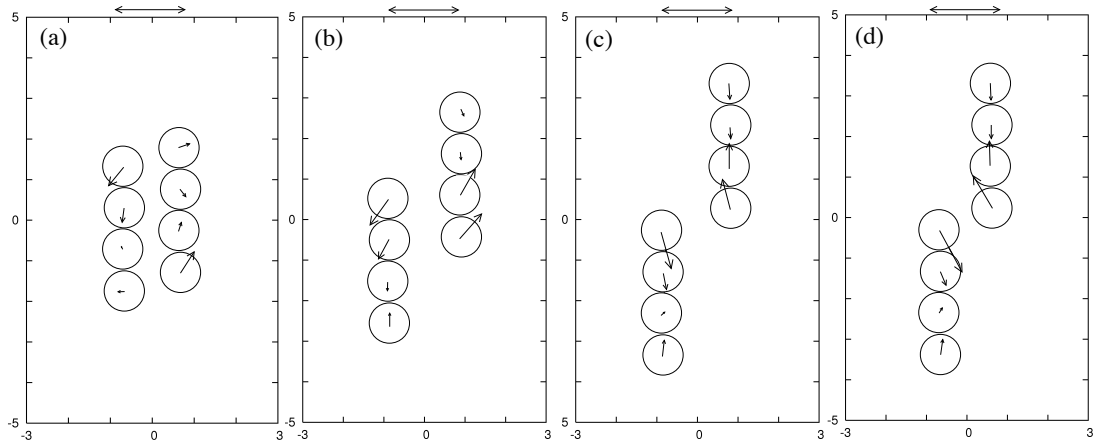


Fig. 6.8: The average forces on each particle for fixed different orientations of two four-particle chains. Illustrating a possible alignment sequence (a)-(d).

additive: we cannot determine the correct magnitude of the forces on short chains from knowledge of the forces between two spheres in isolation. The hypothetical sequence resembles the observations from experiment and simulation in earlier sections.

In order to test the force measurements further we have run simulations in which two four-particle chains are free to move within an oscillated, fluid-filled cell. A series of snapshots are shown in Fig. 6.9. Initially, the two small chains are placed almost parallel to each other in the x - y plane, aligned perpendicular to the direction of oscillation. Each chain remains intact and moves as if it were a single object. The chains “slide” past each other in the y -direction and move slightly further apart. Eventually the nearest ends of each chain attract each other and join together to form one longer chain. This behaviour is consistent with the streaming flow for a short chain shown in Fig. 6.6. The trajectory followed by the chains is similar to that followed by two spheres when forming a pair.

The process of chain interaction continues until the chain becomes full and spans the cell, or there are no more free particles or chains in its vicinity.

6.3.2 Full chains

The addition of particles to a chain continues and short chains get longer. Subsequently the chain is attached to a wall and as more particles attach to the free

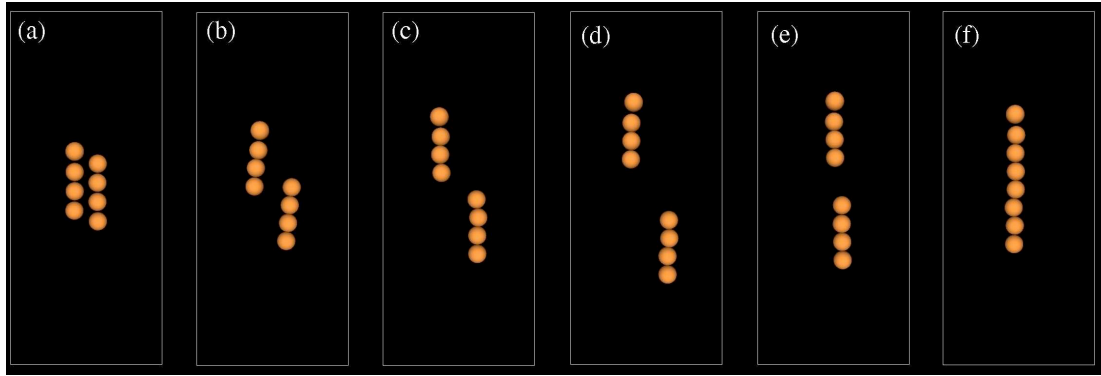


Fig. 6.9: A sequence of snapshots from a simulation showing the formation of a single chain from two shorter chains. The times are (a) 0s, (b) 0.2s, (c) 0.3s, (d) 0.5s, (e) 1.4s and (f) 1.7s. Each frame shows a small part of the simulated area.

end, it can form a full chain which spans the width of the cell. In both simulation and experiment these full chains are stable. The streaming flow for a full chain, in a plane through the centre of the spheres, is shown in Fig. 6.10 (a) and (b). In this plane the outer streaming flow is directed away from the chain. The return path lies above the spheres; *there is no return flow in the plane of the spheres*. The ends of the outer vortex loop terminate on the side walls instead of on the bottom surface of the cell, forming a vortex line, parallel to the chain, which spans the cell. This constitutes a drastic change in the structure of the fluid flow. If there is no return flow in the plane of the spheres there is no reason for other particles to be attracted and there is no room to attach to the ends. The flow in x - z plane is the same as for a short chain shown in Fig. 6.7. But the outer vorticity stays on that plane and does not come down to the surface of the spheres.

6.3.3 Interactions between full chains

So far we have focused on the interactions between particles that lead to the formation of full chains. From studying Figs. 6.3 and 6.5, one might suppose that there is also an interaction between full chains, possibly leading to a well-defined spacing. In order to understand the interaction between full chains we have carried out simulations starting with two full chains separated by 2.0 mm, a separation which is small compared to the steady state separation shown in Fig. 6.5 at 13.44s. The cell is oscillated and the particles are free to move

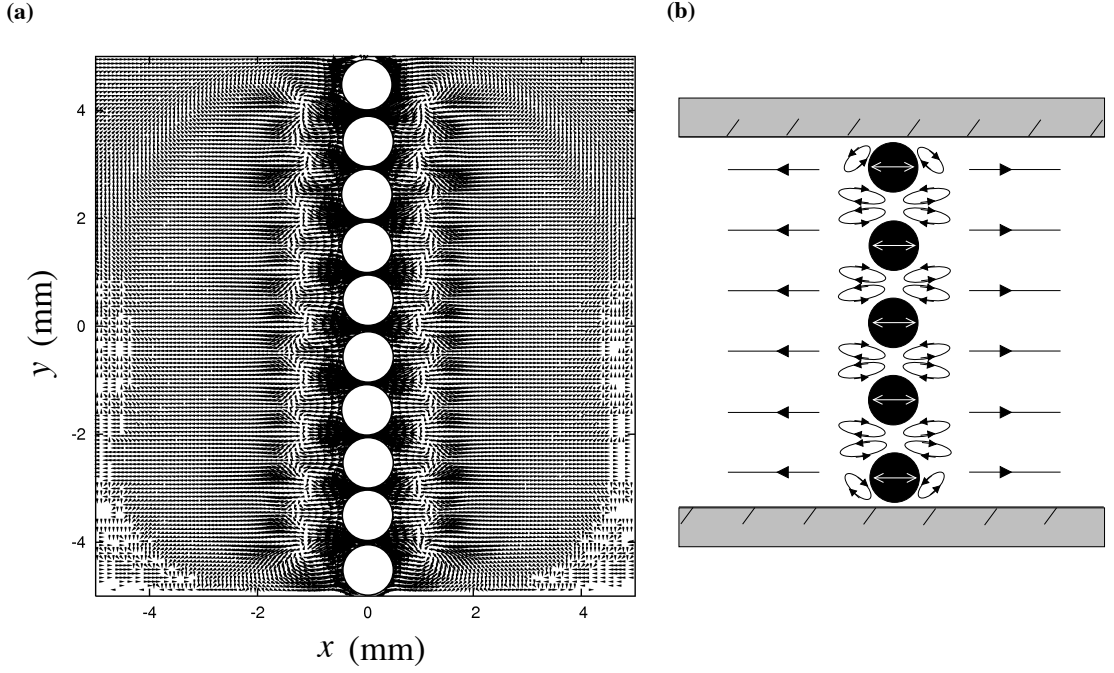


Fig. 6.10: A vector plot taken from simulation (a) and a schematic diagram (b) showing the streaming flow in an x - y plane through the centres of the spheres for a full chain which spans the cell — in (b) we have only shown five spheres for clarity. The vortex loops are parallel to the chain and end at the walls rather than on the bottom surface as they did in Fig. 6.6. The double arrowed line on each sphere indicate the direction of oscillation.

in response to the oscillation. We observe that the chains remain intact but drift apart. Their mean separation as a function of time is shown in Fig. 6.11. The separation between the chains increases with time which suggests that the interaction between chains is solely repulsive.

The repulsive interaction that we observe may be traced to the streaming flow generated by a single full chain, illustrated in Fig. 6.10. In the plane of the spheres, the flow is always away from the chain; there is no return flow in this plane. It is the flow away from the spheres which tends to push the chains apart. In Fig. 6.12 the flow for two full chains is shown at a separation of 6mm.

Further evidence for the existence of a repulsive force due to streaming flows can be obtained by measuring the time-averaged force between full chains that are held at a fixed separation. This method is analogous to the force measurement between two single spheres described in Chapter 5. The mean force on each chain, F_x , is shown in Fig. 6.13. The force is always repulsive but decreases rapidly with separation, D . The solid line is an approximate asymptotic fit showing that

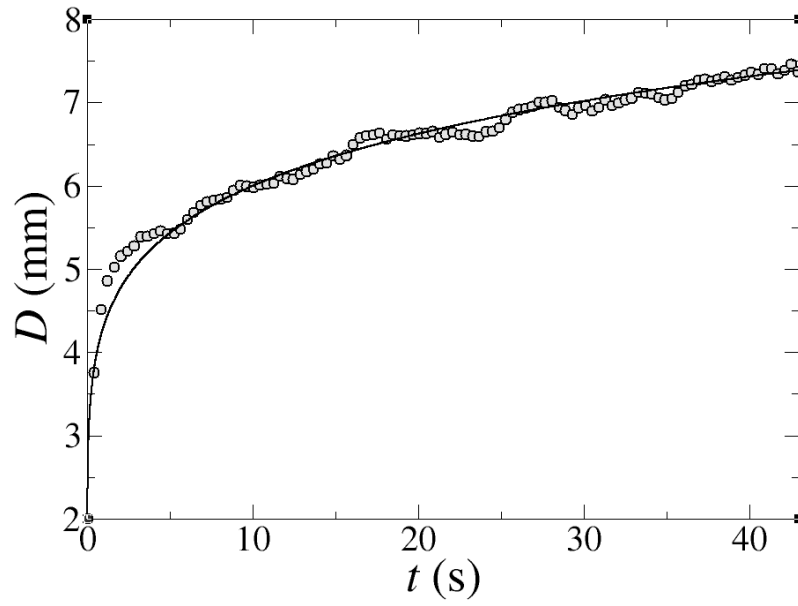


Fig. 6.11: The mean separation between two full chains as a function of time. The points are from simulations and the line is the theoretical fit discussed in the text.

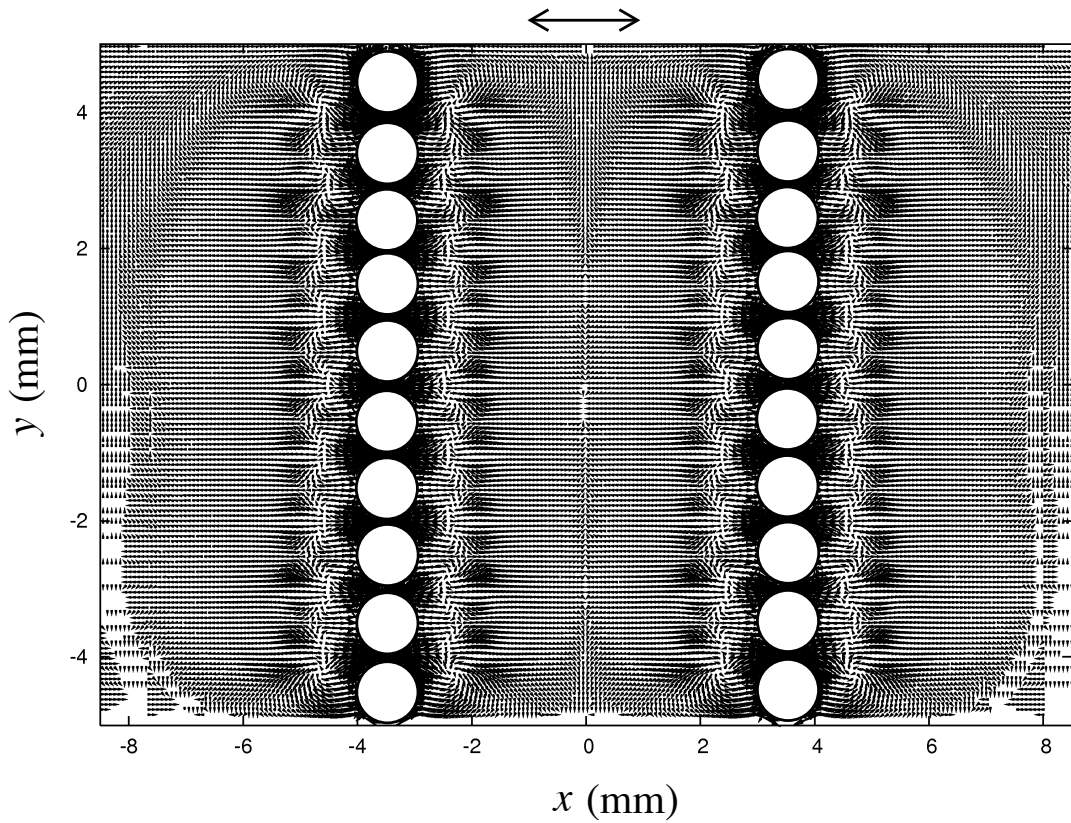


Fig. 6.12: A vector plot taken from simulation, showing part of the time-averaged fluid flow around two full chains. The chains are oscillating in the x -direction and the fluid flow in the x - y plane passing through the centre of the spheres is shown.

$$F_x \sim D^{-6}.$$

The calculation of the time-averaged force assumes that the relative position of the chains is fixed. If the motion of the chains is sufficiently slow, we can use this force to determine their motion. In this limit, the acceleration of the chains is small so that we can ignore inertial effects. The separation, D , obeys an over-damped equation of motion,

$$\alpha \frac{dD}{dt} = 2F_x, \quad (6.1)$$

where F_x is the time-averaged force shown in Fig. 13 and α is an effective drag coefficient. Since we expect this approximation to be valid only for large separations, we have used the asymptotic form

$$F_x \simeq 1300D^{-6}, \quad D \text{ in mm.} \quad (6.2)$$

which is shown in Fig. 6.13 as the solid line. By solving the differential equation we can fit the predicted separation to the data and estimate the effective drag force on each chain in the following way. Substitute F_x from Eq.(6.2) into Eq.(6.1).

$$\alpha \frac{dD}{dt} = 2 \times 1300D^{-6},$$

$$\frac{dD}{dt} = KD^{-6} \quad \text{where} \quad K = \frac{2600}{\alpha},$$

$$\int D^6 dD = K \int dt,$$

$$D = (7Kt + C)^{1/7}. \quad (6.3)$$

The numerical fit to the data of Fig. 6.11 shown as the solid line, is given by $D = (28000t + 1)^{1/7}$, which is in very good agreement with the simulated motion for times greater than 5s, where the velocity and acceleration are small. Comparing with the analytic solution Eq. 6.3 we can get an estimate for the effective drag coefficient α which comes out to be $\alpha = 6.5 \times 10^{-4} \text{ N m}^{-1}\text{s}$.

Differentiating Eq. (6.3) we can also calculate the constant velocity of the chain,

$$\frac{dD}{dt} = \frac{1}{7}(7Kt + B)^{-6/7} \times 7K = 4000(28000t + 1)^{-6/7}, \quad (6.4)$$

at large times, for example $t=42\text{s}$ the velocity of the chain is equal to $\simeq 0.025\text{mm s}^{-1}$. Note that we get the same answer if we calculate the velocity directly from Eq.(6.2) substituting a D to be a large separation, say $D=7\text{mm}$. We can therefore get an estimate for the Reynolds number in steady flow for a chain of spheres, $\text{Re}=uL/\nu$. Substituting the velocity for one chain $u=0.025\times 10^{-3}\text{ms}^{-1}$, the characteristic length L to be the length of the chain we get $\text{Re}=0.1375$ which is within the Stokes limit.

With this estimate for the drag coefficient we can look up how it compares with characteristic values. Let us assume steady Stokes flow. At low Reynolds numbers, in steady flow, the Stokes drag coefficient for a sphere is $C_{\text{sphere}}=6\pi\nu\rho r$. The Stokes drag for one of the spheres of the chain is equal to $C_{\text{sphere}}=1.88\times 10^{-5}\text{ N m}^{-1}\text{s}$.

The drag coefficient for a cylinder in an infinite fluid is given by

$$C_{\text{cylinder}} = 2\pi\nu\rho L \frac{2}{\log(7.4/\text{Re})}, \quad (6.5)$$

where L is the length of the cylinder. If a chain were to be approximated by a cylinder of the same length as the chain then $C_{\text{cylinder}}=1.6\times 10^{-4}\text{ N m}^{-1}\text{s}$. Comparing the drag coefficient for the cylinder with our estimate for α which was $6.5\times 10^{-4}\text{ N m}^{-1}\text{s}$, we see that our value is higher but within the same order of magnitude. Note that the value for the cylinder drag assumes a cylinder in an infinite fluid whereas the chain of the spheres we are studying is of course not a cylinder but a chain of spheres which is on a surface and whose ends are touching the walls of the container. The reasonable agreement between these numbers gives further support to the hypothesis that the repulsive force is due to streaming flows.

6.4 Effect of initial conditions, amplitude and container size

We would like to address the following issues: the effect that the initial conditions, the amplitude and the size of the container have in the formation of chains.

We have carried out some simulations in which the spheres start clustered in

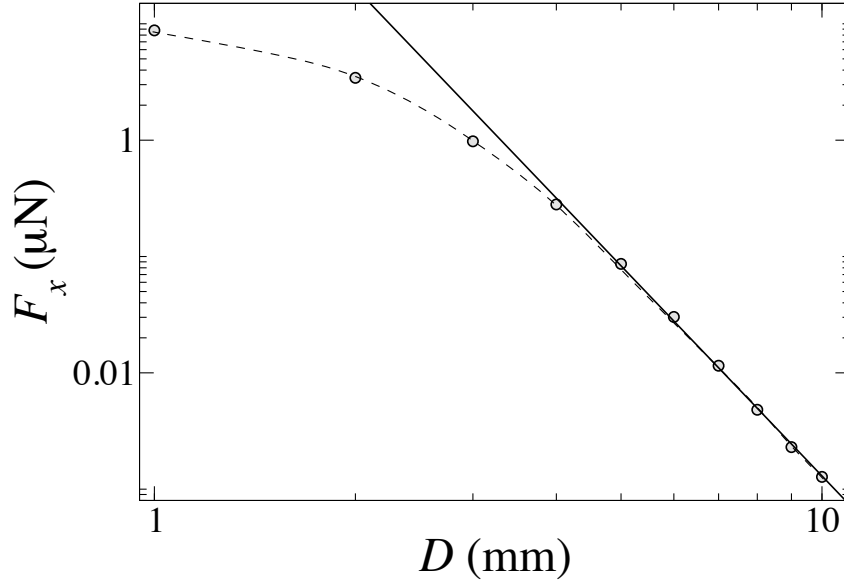


Fig. 6.13: The time-averaged repulsive force between two full chains as a function of their separation. The solid line shows the asymptotic dependence of the force, as discussed in the text. The dashed line is a guide to the eye.

the centre of the cell. Full chains rapidly form and subsequently slowly spread throughout the whole cell due to the weak repulsive interaction. The final configuration is close to that obtained starting from a fully dispersed distribution of spheres, as can be seen in Fig. 6.14 at $t=20.00\text{s}$. The parameters are the same as before, $f=50\text{Hz}$, $A_r=0.5\text{mm}$ and $\nu=2.0 \times 10^{-6}\text{m}^2\text{s}^{-1}$. The only difference is the initial configuration.

In Fig. 6.15 we show a few snapshots for the formation of chains when the frequency and the amplitude are varied. In (a) the frequency is 50Hz and the amplitude is $A_r=0.3\text{mm}$ and in (b) the frequency is 40Hz and the amplitude is $A_r=0.6\text{mm}$. In both (a) and (b) the viscosity is $\nu=2.0 \times 10^{-6}\text{m}^2\text{s}^{-1}$. Again, the final configurations for both (a) and (b) consist of more-or-less evenly spread out chains.

If the container is longer, in the x -direction, then more chains form repelling each other, finally occupying the whole cell. If the container is wider, in the y -direction, fewer chains form also repelling each other, so the distance between neighbouring chains increases, as shown in Fig. 6.16. In all cases, the spatial separation of chains is determined by the geometry of the cell and the number of particles.

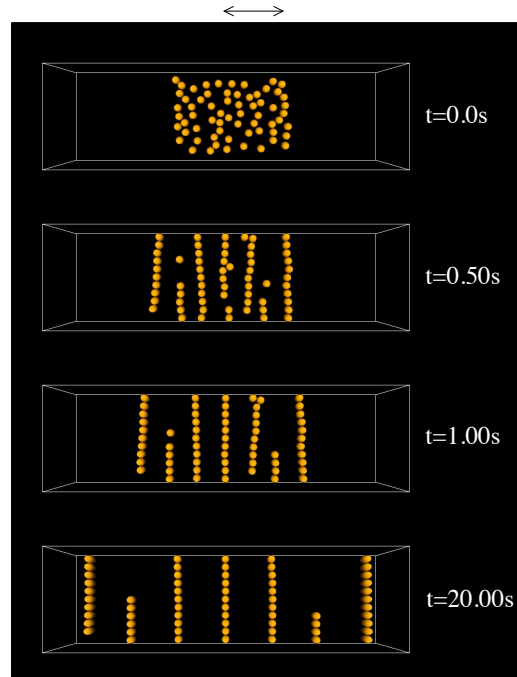


Fig. 6.14: A sequence of snapshots from a simulation showing the formation and evolution of chains from an initially clustered configuration in the middle of the cell.

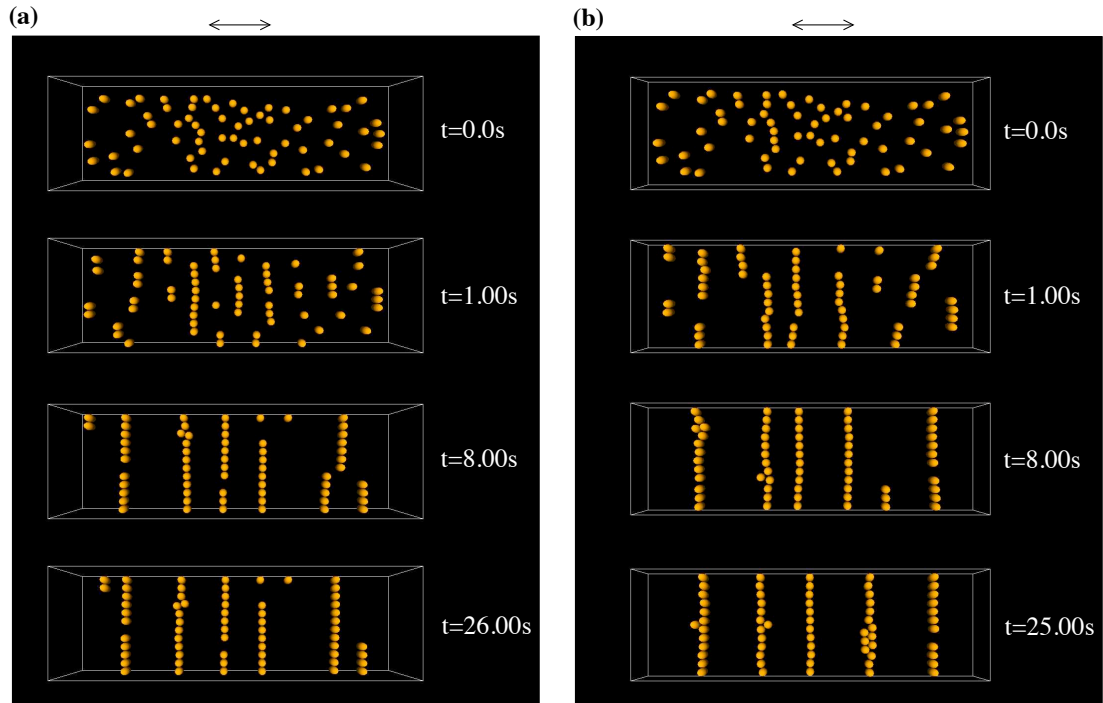


Fig. 6.15: A sequence of snapshots from a simulation showing the formation and evolution of chains when (a) $f=50\text{Hz}$, $A_r=0.3\text{mm}$ and (b) $f=40\text{Hz}$, $A_r=0.6\text{mm}$. In both (a) and (b) the viscosity is $\nu=2.0 \times 10^{-6}\text{m}^2\text{s}^{-1}$.

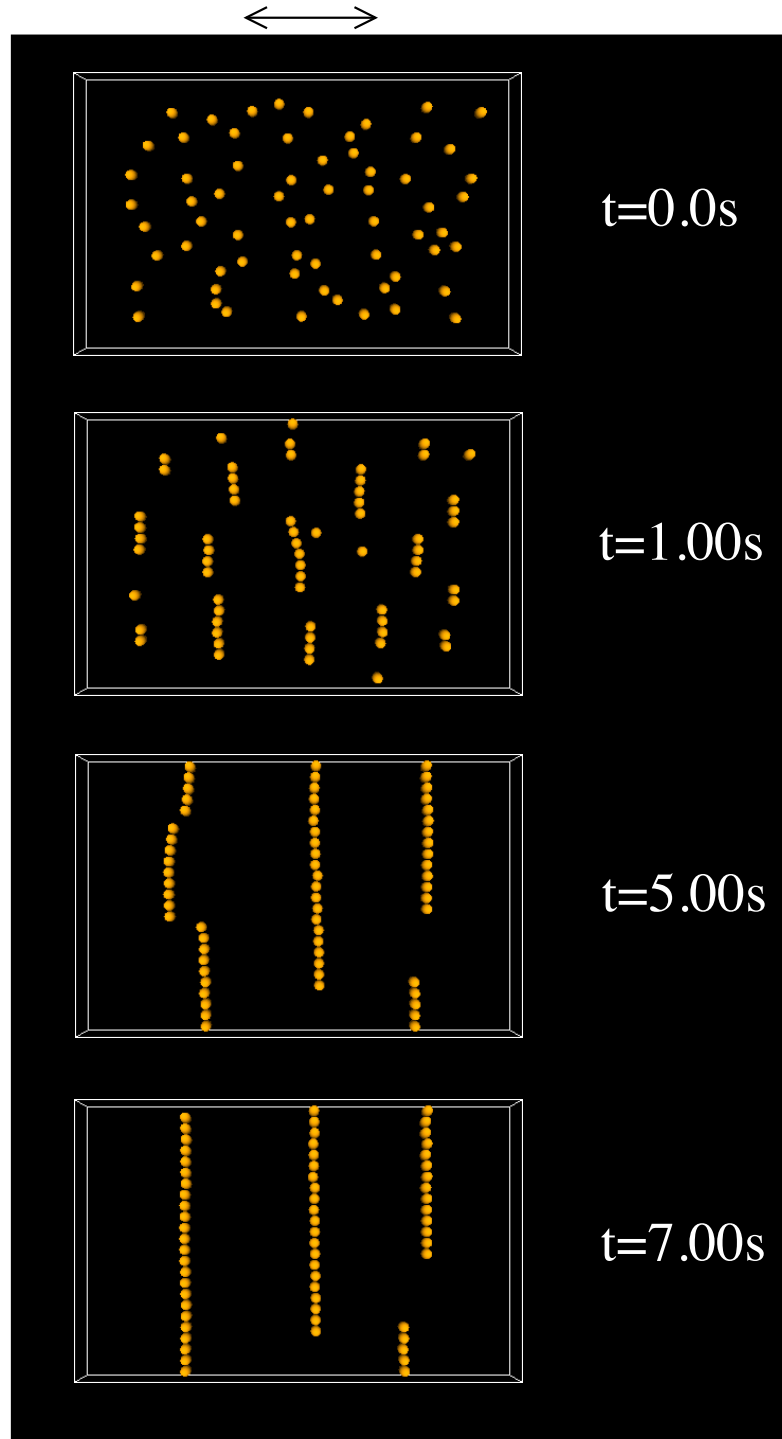


Fig. 6.16: A sequence of snapshots from a simulation showing the formation and evolution of chains for $f=50\text{Hz}$, $A_r=0.5\text{mm}$ and $\nu=2.0 \times 10^{-6}\text{m}^2\text{s}^{-1}$ in a container which is twice as long in the y -direction compared to the container of Figs. 6.14 and 6.15.

6.5 Discussion

We have described in detail the evolution of the system from a collection of single particles to a configuration of stable chains. From Figs. 6.2, 6.3 and 6.4, 6.5 it appears that there is a well-defined separation of chains in the final state of the system. The simplest explanation for a periodic pattern would be the existence of a long-ranged attraction between chains and a short-ranged repulsion. However, in our simulations we were unable to identify an attraction between full chains.

Our explanation of the spacing between the chains in our simulations comes from the fact that individual chain formation is a local ordering phenomenon: each chain is formed from particles in its immediate vicinity. If the initial distribution is on the average spatially homogeneous then the resulting chain structure will appear to be periodic, as in Figs. 6.3 and 6.5. On longer timescales, we have shown that two full chains repel each other weakly. So, for a large number of particles in a finite box, the full chains that form uniformly in the cell are unable to drift further apart because of the presence of the end walls. Consequently, the chains will be equally spaced and the pattern will remain stable. Further evidence supporting this conclusion comes from the simulations done for different initial conditions and box sizes, where in the final configuration evenly-spaced chains fill the container.

It should be noted that frictional forces with the base of the cell have been neglected in our simulations. Provided the forces between chains are large compared to the frictional forces, this approximation can be justified. However, as the pattern evolves the forces between chains decrease and therefore, at longer time scales the frictional forces may eventually be large enough to stop the pattern evolving further. A detailed investigation of frictional effects for particles on a surface in an oscillating fluid is a challenging problem (Wunenburger *et al.* 2002) and beyond the scope of this present study. However some preliminary simulations and experiments show that a stable pattern of chains may be observed by adding a simple static frictional force. It is difficult to know the form of the frictional force because the spheres are oscillating in one direction and interacting with much weaker forces in the perpendicular direction. Moreover, there is an additional force in the vertical direction, due to the asymmetric streaming flows

in the x - z plane between the sphere and the bottom plate, see Chapter 3. For the formation of chains this force seems to be unimportant as gravity dominates in the vertical direction. However when weak frictional effects are considered, this force may also become relevant, as the slightest lift of the sphere from the bottom surface would alter the magnitude of the frictional force.

We would also like address the question of what happens when the container is very large, in the limit where the spheres are not aware of the presence of no-slip walls. We have run numerous simulations but the particles always drift towards the walls. It is difficult to evaluate this because a very large box is computationally too intensive. What we do see though, if we add static friction in the simulations, is that the interaction between chains once formed are much slower than without friction. We wonder whether during this time the chain pattern as a whole could form an *effective streaming flow* which would then keep it stable as a whole in the middle of the container.

Chapter 7

Concluding remarks

The research presented in this thesis studies the dynamics of fluid-immersed dense spheres which are subjected to horizontal sinusoidal vibration. Chain structures are formed perpendicular to the axis of oscillation. The mechanism behind the formation and evolution of the chains of spheres has been studied in detail. Even though we hope our research has shed some light onto these nonlinear systems it also opens up a plethora of questions for future research and ways for technical improvement.

7.1 Summary

Chapter 1 introduced the field of granular materials. A large number of granular systems occur in the presence of fluid. Various structures and patterns had been observed in vibrated fluid-grain systems. We described two experimental studies (Wunenburger *et al.* 2002, Voth *et al.* 2002) which acted as the motivation for our research. In order to understand the details of particle-laden flows, we introduced the governing equations and a brief classification of flows.

In **chapter 2** we described the computational model which was then used in the rest of the thesis. We aimed to model rigid spheres immersed in a fluid, the spheres being allowed to move and to collide with one another as well as with the walls of the container. The fluid obeyed the 3D Navier-Stokes equations, which for finite Reynolds numbers were solved numerically using the projection method (Höfler and Schwarzer 2000) and finite difference approximations. The coupling

between the rigid spheres and the fluid was achieved using the particle-template model (Kalthoff *et al.* 1997) which does the following: the sphere is assumed to be made of fluid grid points occupying a volume of fluid and at every time-step the force that would be acting on this volume of fluid due to the motion in the surrounding fluid is calculated and applied to a volume with the density of the sphere, which moves with respect to the fluid. The collisions between the spheres and the spheres with the walls of the container were modelled using Soft Sphere Molecular Dynamics methods.

In **chapter 3** we discussed some basic physical concepts related to time-periodic flows of a single oscillating sphere in a fluid. In particular the concept of *steady streaming* which is the non-zero time average of a fluctuating flow at finite Reynolds numbers (Riley 1966), was introduced for the case of a single sphere. We described two recent experiments (Kotas 2007, Otto 2008) where the steady streaming flows were measured and we compared their observations with our simulation results, showing reasonably good agreement for the flow fields. We also compared our simulations with known numerical results (Chang and Maxey 1996, Alassar and Badr 1997) measuring the drag coefficient on a sphere and found qualitative agreement. There is a small numerical discrepancy between the results but we trust that our model captures the behaviour of the system whilst allowing the addition of a large number of rigid spheres which are interacting with one another. This is important because to the best of our knowledge, oscillatory systems with more than one interacting spheres at finite Reynolds numbers have not been simulated before. We then introduced the geometry of the system which will be used in the following chapters for experiments and simulations. More specifically, we simulated a single sphere in a shallow fluid-filled container which was vibrated horizontally. The sphere sinks to the bottom surface due to gravity and the oscillate with respect to the fluid and the container. We discussed the way the flow field generated by the sphere was modified due to the presence of the boundaries of the container. The interaction force on the sphere due to one of the boundaries was calculated and was found to decay with separation from the boundary and also depend on the viscosity and vibratory conditions.

Chapter 4 describes a series of experiments performed for two spheres, under-

going horizontal vibration in a shallow fluid-filled cell. The spheres were observed to align perpendicular to the axis of oscillation and sit at a well-defined distance which we called the equilibrium gap. We carried out experiments for various fluid viscosities and vibratory conditions measuring the equilibrium gap and found that all the gap data collapsed according to one of two scaling regimes at low (LAR) and high amplitudes (HAR) (Klotsa *et al.* 2007). The LAR which included most of the data, was qualitatively the same as the stagnation point distance scaling found experimentally by Kotas *et al.* (2007) for the fluid field around a single isolated oscillating sphere. The intriguing observations and results would be studied in more detail in the following chapter in which the same system was simulated.

In **chapter 5** we used the computational model to simulate the experiments for two spheres presented in Chapter 4. Through simulations, we confirmed the two scaling regimes found experimentally and were also able to go into much more detail. In particular, we measured the interaction force between the two spheres and found a long-ranged attraction and a short-ranged repulsion for different viscosities and vibratory conditions. Through force measurements of the field around one oscillating sphere in the vicinity of another we showed that the only stable position for one sphere to be with respect to another is at right angles to the oscillation. The time-averaged streaming flows were calculated and we found two regimes of fluid flow which corresponded to the equilibrium gap regimes LAR and HAR. We gave a simple explanation to why the spheres align and sit a certain distance apart: the inflow of the outer streaming brings the two spheres together and the inner streaming near the surface of each sphere keeps them apart. More importantly, we found that the outer streaming flow around a pair of spheres at equilibrium resembles that of a single sphere which implied that the pair acts as a single object.

In **Chapter 6** we extended our understanding to the study of multiple-sphere systems through experiments and simulations. We studied the formation and evolution of chains from an initially dispersed configuration. Each step of their evolution towards a stable configuration of chains was investigated in detail. We showed that the spheres align locally across the flow forming pairs and short chains, which then act as single objects attracting more spheres onto their free

ends. When a chain expands across the whole cell it becomes stable. Full chains slowly repel each other and we found no evidence of an attraction between neighbouring chains.

7.2 Discussion

The initial goal of the present study was to understand and link two experiments (Wunenburger 2002, Voth 2002) where pattern formation of spheres in oscillatory fluid flows was observed. Wunenburger *et al.* (2002) carried out experiments in which a large number of heavy spheres under horizontal vibration were found to form chains perpendicular to the direction of oscillation. There was an interaction along a chain and an interaction between neighbouring chains. Independently, Voth *et al.* (2002) performed experiments in a three-dimensional geometry in which spheres were bouncing on a vertically-vibrating base under gravity in a viscous fluid and were observed to form lattices and clusters on a plane perpendicular to the axis of oscillation. We chose a simpler system where the geometry was similar to the shallow fluid-filled cell of Wunenburger *et al.* (2002), under horizontal vibration thus avoiding the effect of gravity and bouncing.

We believe that we have understood the mechanism behind the formation of chains, which are the same as in Wunenburger *et al.* (2002). We discuss the differences. In the experiments of Wunenburger *et al.* (2002), smaller particles were used in a much larger cell, with the particles always initially positioned as a clump in the centre of the cell. They noted that the final separation of chains depended upon the vibratory conditions. By varying the vibratory conditions once a pattern had formed, the separation between chains could be made to increase or decrease. This observation suggested the existence of a long-range attraction between chains, although a mechanism for this attraction still remains unknown, as we were not able to identify one. Our simulations have shown that particles are attracted to the free ends of chains due to the return streaming flows in the plane of the chains. In a large cell, provided the chains are far from the side-walls, their free ends could attract neighbouring chains, holding the pattern together. This may be an explanation for the attraction observed by

Wunenburger *et al.* (2002). It would be interesting to investigate this possibility further by performing experiments in a system which we trust to be completely horizontal.

In the experiments of Voth *et al.* (2002) the set up is different. Yet, by extending our understanding to a three-dimensional flow where the spheres are not sliding on a bottom surface, we would suggest that the observed lattices and clusters are the equivalent of a three-dimensional chain. More specifically, similar to the pairs sitting at an equilibrium gap, there should be a long-ranged attraction due to the outer steady streaming flow, as had already been proposed by the authors, and there should be a short-ranged repulsion due to the inner steady streaming flow. We would also expect that the flow for a cluster of spheres would share the outer streaming flow, thus holding it together as a single object. In the absence of gravity, we would expect layers of spheres to form, each layer at right angles to the vibration axis, in the same way that chains formed under horizontal vibration.

We have seen that the simple computational model we have used has managed to capture the behaviour of the system and even the time-scales for a large number of spheres under horizontal vibrational. However, there is a dependence on the grid spacing of the lattice, in other words the resolution, the number of points that make up the sphere. In steady flows the error is very small and we have achieved very good agreement for the drag coefficient in a Reynolds number range 1-500. In oscillatory flows however the error is bigger. As the resolution becomes finer quantities such as the oscillatory drag coefficient also become more accurate but the computational cost is too intense. A possible way out of this is to use a more elaborate model which depends less on the grid spacing. The complete version of the Fluid-Springs model which uses a spring force to couple the fluid and grain motions would be a good candidate (Höfler and Schwarzer 2000).

Finally we would like to discuss what happens in the same system when we have two spheres which are *not* equal in size. It was observed experimentally that two spheres of different sizes would initially interact in the same way as the pairs attracting each other to a certain distance and aligning perpendicular to the oscillation axis. However, as soon as they are aligned across the flow the

asymmetric pair is observed to migrate in the direction of the smaller sphere at right angles to the oscillation (Wright *et al.* 2008). Wright *et al.* (2008) found that the reason behind the migration of the asymmetric pair, was due to the formation of asymmetric streaming flows which would then generate a force on the pair towards the direction of the smaller sphere. So the generation of steady streaming flows around spheres oscillating at finite Reynolds numbers can induce ordered structure formation such as the chains and lattices which we have seen already but also net motion in a specific direction when asymmetry is introduced. Based on the above findings we wonder whether an internally-vibrated asymmetric object such as a biological or artificial micro-swimmer could move through fluid due to the generation of asymmetric streaming flows.

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