

IMPERIAL

Numerical simulations of environmentally relevant multiphase flows

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Declaration of Originality

This dissertation is a description of the work carried out by the author in the Department of Chemical Engineering, Imperial College London, under the supervision of Prof. Omar K. Matar. Except where acknowledged, the content is the original work of the author and no portion of it has been submitted in support of an application for a degree at any other university.

I hereby certify that the material in this thesis is the result of my own original research. All consulted materials have been properly acknowledged and the literature used has been referenced.

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Abstract

The accumulation of marine debris has become an environmental challenge, threatening marine ecosystems and coastal communities. The abundance of plastic debris in the ocean serves as the motivation for the work carried out in this thesis. The focus of this thesis is on the transport of particles in inhomogeneous fluids, as it is important to gain an understanding of what happens at the particle scale to help combat marine pollution. In the ocean, ambient stratification caused by salinity or temperature gradients can play a crucial role in the transport and fate of microplastics. In this thesis, our in-house solver, *BLUE*, is used to perform direct numerical simulations of particle transport and interactions in homogeneous and density-stratified fluids.

Firstly, an investigation on the effect of ambient fluid stratification on the vertical transport of particles with different geometries is performed, benchmarking the results against the literature. Furthermore, this thesis considers the rising dynamics of perforated discs in both homogeneous and density-stratified fluids, where the results present the effect of stratification and perforations to suppress the fluttering dynamics otherwise found for impervious discs in homogeneous fluids. A pairwise interaction study of spheroids with varying aspect ratios is also conducted at low Reynolds numbers, drawing comparisons to the behaviour of spheres under similar conditions. Increasing the particle count to a sparse cluster of spheres is then examined to assess how ambient fluid stratification influences the temporal evolution of the cluster variance opposed to its homogeneous counterpart. Lastly, microplastics in the ocean are susceptible to bubble scavenging, in which rising bubbles capture suspended particles by attaching to the air/water interface and carrying them upward. In the last chapter, we consider the interaction between a rising bubble and a settling sphere of a similar size, investigating the role of the dimensionless numbers, which characterise the flow.

Acknowledgements

I dedicate this work to my family: my mother, Majda, and my late father, Mahdi, for the love, guidance, and sacrifices that have shaped my life. I also dedicate it to my uncle, Hameed, for his care, support, and presence throughout the years. I further dedicate it to my brothers and sister, Abdulhameed, Abdullateef, and Bebe, for their constant support, patience, and encouragement, especially during the years I have been away from home. Everything I have achieved has been built on what you have given me, and I will always be grateful.

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Dedication

To my family,
for their love and support.

Scientific output

Listed below are the manuscripts in which I participated during my PhD that form the foundation of this thesis:

1. **A. M. Abdal**, D. Panda, L. Kahouadji, M. Shams, S. Shin, J. Chergui, D. Juric, and O. K. Matar. ‘Numerical simulations of annular disc dynamics in homogeneous and density-stratified fluids at moderate Reynolds number’. *Under Revision, **Phys Rev Fluids***.
2. **A. M. Abdal**, L. Kahouadji, S. Shin, J. Chergui, D. Juric, C. P. Caulfield, and O. K. Matar. ‘Pairwise interaction of in-line spheroids settling in a linearly stratified fluid’. *Acta Mechanica* (Special Issue), 2024. <https://doi.org/10.1007/s00707-024-04125-4>.
3. **A. M. Abdal**, L. Kahouadji, S. Shin, J. Chergui, D. Juric, C. P. Caulfield, and O. K. Matar. ‘On the interaction between a rising bubble and a settling particle’, *J Fluid Mech*, (2024). <https://doi.org/10.1017/jfm.2024.686>.

Listed below are the additional publications in which I participated during my PhD:

4. **A. M. Abdal**, D. Panda, L. Kahouadji, M. Shams, S. Shin, J. Chergui, D. Juric, and O. K. Matar. ‘Three-dimensional numerical simulations of product changeover: Miscible and immiscible displacements in circular tubes’. *Int J Multiphase Flows*, 2026. <https://doi.org/10.1016/j.ijmultiphaseflow.2026.105634>.
5. M. Shams, D. Panda, **A. M. Abdal**, L. Kahouadji, S. Shin, J. Chergui, D. Juric, and O. K. Matar. ‘Self-similar pinch-off in surfactant-laden flows in a capillary tube’, *J Fluid Mech*, 2026. <https://doi.org/10.1017/jfm.2026.11583>.
6. D. Panda, S. Shin, **A. M. Abdal**, L. Kahouadji, J. Chergui, D. Juric, and O. K. Matar. ‘Direct numerical simulation of two-phase flows with surfactant-induced

surface viscous effects’. *J Comp Phys*, 2026. <https://doi.org/10.1016/j.jcp.2026.114914>.

7. L. Kahouadji, D. Panda, M. Shams, **A. M. Abdal**, S. Shin, J. Chergui, D. Juric, and O. K. Matar. ‘The crown: Rolling splash’. *Phys Rev Fluids*, GFM 2025. <https://doi.org/10.1103/t2zw-4577>.
8. D. Panda, L. Kahouadji, **A. M. Abdal**, S. Shin, J. Chergui, D. Juric, L. Tuckerman, and O. K. Matar. ‘Drop Medusa: Direct numerical simulations of high-frequency Faraday waves on spherical drops’. *Phys Rev Fluids*, GFM 2024. <https://doi.org/10.1103/PhysRevFluids.9.110514>.
9. D. Panda, **A. M. Abdal**, M. Shams, L. Kahouadji, J. Chergui, S. Shin, D. Juric, and O. K. Matar. ‘Interfacial standing wave-patterns disentangle dilatational and shear surface viscous effects’, *Under revision*, *Communications Phys*. <https://doi.org/10.48550/arXiv.2601.06881>.

Lastly, below are the manuscripts currently under preparation from work in which I participated during my PhD:

10. D. Panda, Nicolas Perinet, L. Tuckerman, **A. M. Abdal**, L. Kahouadji, S. Shin, J. Chergui, D. Juric, and O. K. Matar. ‘Hexagonal pattern transitions and superlattices in two-frequency parametric surface waves’. *To be submitted to Phy Rev E*.

Some of the work during my PhD has also been disseminated in the following international conferences, where the asterisk denotes the presenter:

1. **A. M. Abdal***, L. Kahouadji, S. Shin, J. Chergui, D. Juric, C. P. Caulfield, and O. K. Matar. ‘Direct numerical simulations of particles settling in a stratified fluid’. 2022 APS-DFD Annual Meeting. Remote presentation (November 2022).
2. **A. M. Abdal***, L. Kahouadji, S. Shin, J. Chergui, D. Juric, C. P. Caulfield, and O. K. Matar. ‘Direct numerical simulations of bubble-particle interactions’. 2023 APS-DFD Annual Meeting. Washington D.C., USA (November 2023).
3. **A. M. Abdal***, L. Kahouadji, S. Shin, J. Chergui, D. Juric, and O. K. Matar. ‘Direct numerical simulations of miscible and immiscible displacements in pipelines for product changeover’. 2024 ChemEngDayUk. London, United Kingdom (April 2024). (Poster Contribution).

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4. **A. M. Abdal***, L. Kahouadji, S. Shin, J. Chergui, D. Juric, C. P. Caulfield, and O. K. Matar. ‘Pairwise interactions of settling spheroids in a linearly stratified fluid’. 2024 BIFD. Edinburgh, Scotland (June 2024).
 5. **A. M. Abdal***, L. Kahouadji, S. Shin, J. Chergui, D. Juric, C. P. Caulfield, and O. K. Matar. ‘Direct numerical simulations of particles settling in a stratified fluid’. 2024 ICTAM. Daegu, South Korea (August 2024).
 6. **A. M. Abdal***, L. Kahouadji, S. Shin, J. Chergui, D. Juric, C. P. Caulfield, and O. K. Matar. ‘Numerical simulations of dilute particle suspensions settling through a density interface’. 2024 EFDC1. Aachen, Germany (September 2024).
 7. **A. M. Abdal***, L. Kahouadji, S. Shin, J. Chergui, D. Juric, and O. K. Matar. ‘Direct numerical simulations of miscible and immiscible displacements in pipelines for product changeover’. 2024 AIChE Annual Meeting. San Diego, California, USA (November 2024).
 8. **A. M. Abdal***, L. Kahouadji, S. Shin, J. Chergui, D. Juric, C. P. Caulfield, and O. K. Matar. ‘Direct numerical simulations of particle suspensions settling in a stratified fluid’. 2024 APS DFD. Utah, USA (November 2024).
 9. S. Shin, **A. M. Abdal***, L. Kahouadji, J. Chergui, D. Juric, C. P. Caulfield, and O. K. Matar. ‘Pairwise interaction of in-line spheroids settling in a linearly stratified fluid’. 2024 APS DFD. Utah, USA (November 2024).
 10. D. Juric, **A. M. Abdal***, L. Kahouadji, S. Shin, J. Chergui, C. P. Caulfield, and O. K. Matar. ‘On the transport of droplets and bubbles through density transition layers’. 2024 APS DFD. Utah, USA (November 2024).
 11. **A. M. Abdal***, L. Kahouadji, S. Shin, J. Chergui, D. Juric, C. P. Caulfield, and O. K. Matar. ‘On the interaction between solid particles settling in a density stratified fluid’. 2025 ICMF. Toulouse, France (May 2025).
 12. M. Shams, D. Panda, **A. M. Abdal***, L. Kahouadji, S. Shin, J. Chergui, D. Juric, and O. K. Matar. ‘Direct numerical simulation of contact-line-driven dewetting and pinch-off dynamics in surfactant-laden flows’. 2025 APS DFD. Texas, USA (November 2025).
 13. **A. M. Abdal***, D. Panda, L. Kahouadji, M. Shams, S. Shin, J. Chergui, D. Juric, C.P. Caulfield and O. K. Matar. ‘Settling of perforated discs in a density-stratified fluid’. 2025 APS DFD. Texas, USA (November 2025).

Contents

1	Introduction	1
1.1	Motivation and scope	2
1.2	Thesis outline	6
2	Literature review	7
2.1	Governing physics	8
2.2	Particle dynamics in homogeneous fluids	11
2.3	Boussinesq approximation	16
2.4	Particle dynamics in density-stratified fluids	18
2.5	Particles, drops and bubbles	30
2.6	Summary and remarks	34
3	Numerical framework	36
3.1	Overview	37
3.2	Numerical methods for multiphase flows	37
3.3	Solving the governing equations	50
3.4	Remarks	59
4	On the motion of a particle in a density-stratified fluid	60

4.1	Introduction	61
4.2	Benchmark tests	65
4.3	Simulation Setup	69
4.4	Results and discussion	70
4.5	Concluding remarks	90
5	The role of particle interactions in a density-stratified fluid	92
5.1	Introduction	93
5.2	Benchmark tests	96
5.3	In-line spheroids in a density-stratified fluid	99
5.4	Increasing N_p for spheres	120
5.5	Concluding remarks	130
6	On the interaction between a settling particle and a deformable interface	132
6.1	Introduction	133
6.2	Numerical setup	134
6.3	Results and discussion	141
6.4	Concluding remarks	157
6.5	Resolution tests	159
7	Conclusions and future outlooks	161
	Bibliography	168

List of Figures

1.1	Panel (a) shows a schematic of relevant processes near the ocean surface, adapted from DiBenedetto [3]. Panel (b) shows the plethora of different shapes of plastics found in the ocean, adopted from Sutherland et al. [9].	3
1.2	Panel (a) presents an illustration of the different scales governing the transport of microplastics in the ocean, adopted from Vowinckel [10]. Panel (b) illustrates the inherent density-stratification in the ocean, adopted from More and Ardekani [11].	4
2.1	Panel (a) shows many particles of arbitrary shape in a background flow. Panel (b) depicts a spherical particle with translational velocity $\mathbf{u}_p$ and angular velocity $\boldsymbol{\omega}_p$, and an outward-pointing normal $\mathbf{n}$. Panel (c) illustrates the force balance for a stationary spherical particle and for a spherical particle in motion. The panels are adapted from Guazzelli and Morris [17].	9
2.2	Shape of spheroids when varying the aspect ratio χ . Figure adapted from Will et al. [18].	11
2.3	Panel (a) shows some of the investigated parameter ranges in a three-dimensional parameter space $(\bar{\rho}, Re, \chi)$, and panel (b) presents the critical Re for the onset of instabilities for cylinders of aspect ratio χ . Re_{c1} and Re_{c2} are the steady and Hopf bifurcation of flow past a fixed body, whereas Re_c gives the critical Re for the onset of path instability from the experiments of Fernandes et al. [19]. Empirical fits are also provided in panel (b). The figure is adapted from Ern et al. [20].	13

2.4	Panel (a), adapted from Tinklenberg et al. [21], presents sample trajectories for thin discs falling in air from the experiments of Tinklenberg et al. [21]. The observed regimes correspond to a straight vertical path, a small amplitude fluttering motion, a large amplitude fluttering motion, and a tumbling regime. Panel (b), adapted from Vincent et al. [22], presents the regime map for falling discs from Field et al. [23], describing the different regimes based on (Re, I) parameter space, but including the role of a central perforation on the dynamics (effect of d_i/d_o).	14
2.5	Panel (a) shows the simulations of Zhang et al. [14] for a settling sphere in a linearly stratified fluid and changing the underlying dimensionless numbers. Panel (b) shows the different wake patterns found for a settling sphere in a linearly stratified fluid from the experiments of Hanazaki et al. [28]. The figure has been adapted from More and Ardekani [11].	20
2.6	Panel (a) shows the levitation behaviour found for a sphere settling through a sharp density transition layer from the experiments of Abaid et al. [29]. In panel (b), the flow field of a sphere settling in a linearly stratified fluid is presented highlighting the vorticity profile and the distorted isopycnals from the simulations of Doostmohammadi et al. [30]. In panel (c), a regime map for the settling behaviour from the simulations of Doostmohammadi et al. [30] is presented when $(Re = 353, Sc = 700)$ and varying Fr . The figure is adapted from More and Ardekani [11].	21
2.7	An illustration of the reorientation behaviour of a settling spheroid in a linearly stratified fluid is presented in panel (a), as seen from the work of More et al. [35]. In panel (b), an illustration of the interaction between a spherical particle pair in a homogeneous and density-stratified fluid is presented in both the side-by-side and in-line configurations. The figure is adapted from More and Ardekani [11] and Ardekani et al. [36].	24

- 2.8 Panel (a) shows a Hadamard–Rybczynski type toroidal circulation throughout the particle cloud volume, with the moving reference frame streamlines. In panel (b), the disintegration of a particle cloud into a torus, and further into daughter droplets in a cascade is presented. Panels (a) and (b) are adapted from Guazzelli and Morris [17] and Guazzelli [43], respectively. A top view spatio-temporal evolution of the interaction between spherical particles initialised as a sparse cluster is presented in panel (c) from the experiments of Daniel et al. [44] with $N_p = 20$ and $Re = 93$, where N_p is the number of particles. In panel (d), the spatio-temporal evolution of a spherical particle cluster of neutrally buoyant particles in a sharply stratified fluid from the experiments of Camassa et al. [45], highlighting their self assembly. 26
- 2.9 Growth exponents for the evolution of spherical particle cluster where $\langle r_t^2 \rangle = t^\alpha$ when varying N_p and Re from the experiments of Daniel et al. [44]. The solid line corresponds to $\alpha = 2/3$, and the marker shapes are: $Re = 93$ ($\diamond$), $Re = 216$ ($\square$), $Re = 425$ ($\triangle$). 28
- 2.10 Regime map characterising the dynamics of a rising bubble in a homogeneous fluid when varying (Bo, Ga) . The regime map is adopted from Tripathi et al. [60]. The regimes are: (I) an axisymmetric bubble at small Ga and small Bo ; (II) a spiralling bubble at large Ga and small Bo ; (III) a skirted spherical-cap bubble at small Ga and large Bo ; and, at large Ga and large Bo , (IV) peripheral breakup or (V) central breakup. 31
- 3.1 Panel (a) shows the three-dimensional Eulerian grid structure with the phase interface, panel (b) presents a schematic of the LCRM in two-dimensions, and panel (c) shows the subdivision of tetrahedral cells in three-dimensions with the tetra-marching procedure for continuous interface interconnection. Figures are adapted from Shin et al. [108]. . . . 42
- 3.2 Panel (a) shows an illustration of the notation utilised for the collision model. In panel (b), a comparison of the collision model with the experimental results of Gondret et al. [127] for a solid sphere bouncing off a solid wall is provided. Two different initial separation distances were considered, and they are $\xi_{in} = 1.4D_p$ and $\xi_{in} = 0.43D_p$. For these two initial separation distances, four restitution coefficients were tested, ranging between $e = [0.68, 0.98]$ 49

4.1	Schematic of the disc geometry. The coordinate system, gravity direction, and inclination angle θ between the disc normal $\mathbf{n}$ and the vertical z axis are shown. Side and top views compare a solid disc and a perforated disc of outer diameter D_D and thickness h , with a central hole of diameter d	63
4.2	Validation of the numerical technique: comparison of the temporal evolution of the particle settling velocity in a homogeneous fluid obtained from numerical method and published experimental data; (a) and (b), and (c) show results for $Re = 11.6$ and 31.9 [147], and $Re = 41$ [148], respectively.	65
4.3	Panel (a) presents a comparison with the results of Doostmohammadi et al. [30] (markers) for a sphere settling in a linearly stratified fluid with $Re = \rho_{f,0}U_s D_p / \mu_f = 14.1$ and different Fr , where U_s is the Stokes settling velocity. Panel (b) shows the corresponding flow field for a spherical particle settling in a linearly stratified fluid at fixed $Sc = 700$ and $Fr = 6$, for two Reynolds numbers, $Re = 0.15$ and $Re = 10$. The left subpanels show the isopycnals, while the right subpanels show glyphs of the velocity field. Panel (c) shows the variation of the dimensionless perturbed density $\rho^* = (\rho_f - \rho_f _{z=z_{\text{peak}}})/(\gamma D_p)$ along the horizontal $z = z_{\text{peak}}$ plane near the sphere at peak particle velocity for $Re = 14.1$, $Fr = 1.62$, $Sc = 700$	66
4.4	Panel (a) presents sample flow fields in the vicinity of a settling sphere in a linearly stratified fluid as the Schmidt number Sc is varied, with $Re = \rho_{f,0}U_s D_p / \mu_f = 14.1$ and $Fr = 1.62$, where U_s denotes the Stokes settling velocity. Panel (b) shows the corresponding particle velocity profiles for these cases, compared with the results of Doostmohammadi et al. [30] (markers).	67

- 4.5 Panel (a) shows the Reynolds number against the Archimedes number for rising discs in a homogeneous fluid. The computational results are presented against the experimental results of Fernandes et al. [154] for various aspect ratios χ . The solid line corresponds to $C_D^H = 1.2$. Panel (b) compares the drag coefficient C_D^H from the simulations to empirical correlations and experimental measurements [155]. The inset shows two sample volume renderings of the vorticity profile for an impervious and perforated disc with $d/D_D = 0.5$ ($Ar = 90$, $\chi = 7$). The unfilled red markers correspond to the simulation results with solid discs, and the filled red markers correspond to perforated discs with $d/D_D = 0.5$ 71
- 4.6 Disc trajectory in the x - z plane (side view), time histories of the vertical (V_z , solid) and lateral (V_x , dashed) velocities, and the inclination angle θ shown for $Ar = 90$, $\chi = 7$, and $Ar = 49$, $\chi = 7$ in (a) and (b), respectively. Here, $I^* = 0.0072$ for solid discs, and $I^* = 0.0067$ for perforated discs. 72
- 4.7 Time histories of the disc lateral velocity V_x (solid lines) and angular velocity $\dot{\theta}$ (dash-dotted lines) for $Ar = 49$ and $\chi = 7$, with varying d/D_D . The corresponding dimensionless moments of inertia are $I^* = [0.0072, 0.0071, 0.0067]$ for $d/D_D = [0, 0.25, 0.5]$, respectively. 73
- 4.8 Spatio-temporal evolution of the vorticity profiles ω_y in the x - z plane with $Ar = 90$, $\chi = 7$ for a solid disc in panel (a) and a perforated ($d/D_D = 0.5$) disc in panel (b). The time history spans $tU/R_{eq} = 30$ to $tU/R_{eq} = 100$, with snapshots taken at intervals of $\Delta t = 10$. The results are shown on a slice in the y -normal direction, with a height of $9D_D$, extending from $1.8D_D$ above the disc to $7.2D_D$ below the disc. 75
- 4.9 Panel (a) shows a close up comparison of the vorticity profile and the body frame streamlines with $Ar = 90$, $\chi = 7$ for a solid and perforated disc ($d/D_D = 0.5$) at $tU/R_{eq} = 30$. The colour map is the same as Fig. 4.8. The time history of the circulation Γ is presented in panel (b), where the inset illustrates the contributions to Γ for either case. 76

- 4.10 Disc trajectory in the x - z plane, time histories of the vertical (V_z , solid) and lateral (V_x , dashed) velocities, and the inclination angle θ for $Ar = 90$, $\chi = 7$, $Fr = 17$, $Sc = 0.7$, and $Ar = 49$, $\chi = 7$, $Fr = 17$, $Sc = 0.7$ shown in (a) and (b), respectively. Here, $I^* = 0.0072$ for solid discs, and $I^* = 0.0067$ for perforated discs. 78
- 4.11 Spatio-temporal evolution of the vorticity profiles ω_y in the x - z plane with $Ar = 90$, $\chi = 7$, $Fr = 17$, $Sc = 0.7$ for a solid disc in panel (a) and a perforated ($d/D_D = 0.5$) disc in panel (b). The time history spans $tU/R_{eq} = 30$ to $tU/R_{eq} = 150$, with snapshots taken at intervals of $\Delta t = 60$. The results are shown on a slice in the y -normal direction, with a height of $9D_D$, extending from $1.8D_D$ above the disc to $7.2D_D$ below the disc. 79
- 4.12 Panel (a) shows side views in the x - z plane of the wakes for a solid disc and a perforated disc with $d/D_D = 0.5$ in the stratified cases at $Ar = 90$, $\chi = 7$, $Fr = 17$, and $Sc = 0.7$ at $tU/R_{eq} = 150$. The axes are normalised by D_D and are with respect to the centre of mass of the disc. The left side presents the distorted isopycnals, and the right side shows the laboratory frame streamlines. Panel (b) shows the temporal evolution of the enstrophy ζ , and the buoyancy flux $\mathcal{B}$ 80
- 4.13 Panel (a) shows the centreline profile of the relative wake vertical velocity $V_z^f/V_z - 1$ as a function of z_{rel} , the vertical coordinate measured relative to the disc centre at its instantaneous height, for $Ar = 90$, $\chi = 7$, $Fr = 17$, and $Sc = 0.7$ at $tU/R_{eq} = 90$ and $tU/R_{eq} = 150$. Markers indicate the relative vertical position z_{rel} at which V_z^f attains its minimum. Circles correspond to $tU/R_{eq} = 90$, and squares correspond to $tU/R_{eq} = 150$. Panel (b) shows the lateral profile of V_z^f along the x direction evaluated at these marker locations. 81

- 4.14 Panel (a) shows side views in the x - z plane of the wakes for a solid disc and a perforated disc with $d/D_D = 0.5$ in the stratified cases at $Ar = 49$, $\chi = 7$, $Fr = 17$, and $Sc = 0.7$ at $tU/R_{eq} = 150$. The axes are normalised by D_D and are with respect to the centre of mass of the disc. The left side presents the distorted isopycnals, and the right side shows the laboratory frame streamlines. The body frame streamlines are presented at $tU/R_{eq} = 150$, and a plot of the relative fluid velocity $V_z^f/V_z - 1$ is presented at two different time steps. Panels (b) and (c) correspond to $(Sc = 7, Fr = 17)$ and $(Sc = 7, Fr = 11.4)$, respectively. 83
- 4.15 Time histories of the disc's instantaneous vertical position are shown for (a) $Ar = 49$ at $Fr = 17$ with $Sc = 0.7$ and $Sc = 7$, for both $d/D_D = 0$ and $d/D_D = 0.5$, and (b) $Ar = 49$, $Sc = 7$, $Fr = 11.4$ for $d/D_D = 0$, 0.25 , and 0.5 . Panel (c) shows the corresponding rise trajectories for the cases in panel (b). 84
- 4.16 Spatiotemporal evolution of the vorticity field ω_y for $Ar = 49$, $Sc = 7$, $Fr = 11.4$ when (a) $d/D_D = 0$, (b) $d/D_D = 0.25$ and (c) $d/D_D = 0.5$. From left to right, $tU/R_{eq} = [200, 300, 350, 400, 450]$ 85
- 4.17 Panels (a) and (b) present the time history of $|\theta|$ with respect to V_z/U and $N(t - t_c)/2\pi$, respectively. Here t_c is the time where $\theta = 5^\circ$ during the reorientation process. The dashed line in panel (b) corresponds to $5e^{\sigma N(t-t_c)/2\pi}$, where $\sigma = 2.7$ as per the experiments of Mercier et al. [37]. In panel (c), the phase diagram of the angular velocity and the orientation angle is presented, where the dashed line has a slope of $\sigma/2\pi$. The results here correspond to $Ar = 49$, $Sc = 7$, $Fr = 11.4$ and varying d/D_D 87

- 4.18 Panel (a) presents a force decomposition (z -direction) from $tU/R_{eq} = 25$ to $t = t_c$ when $Ar = 49$, $Sc = 7$, $Fr = 11.4$, and $d/D_D = 0$, illustrating quasi-steady behaviour. Panel (b) shows the evolution of $C_D^S - C_D^H$ as a function of the instantaneous Froude number $Fr(z)$. The inset in panel (b) presents the instantaneous Reynolds against Archimedes numbers. Under quasi-steady state, $C_D^S = \frac{32}{3} \frac{Ar(z)^2}{Re(z)^2}$. The cases in panel (b) are for $Ar = 49$, $Sc = 7$, $Fr = 11.4$ and varying d/D_D . Panel (c) shows the stratification-induced drag enhancement, $(C_D^S - C_D^H) \sqrt{Re(z)/Fr(z)}/(1 + 2/\chi)$, as a function of the instantaneous Froude number $Fr(z)$. The dashed line denotes a power-law fit, $16.5Fr(z)^{-1.4}$ 88
- 5.1 Panel (a) compares our numerical predictions with those of Deepwell et al. [16], for a spherical particle pair settling in a sharply stratified fluid. The simulation setup with the required definitions are provided as an illustration (adapted from Deepwell et al. [16]), and the numerical results for the angle ϕ between the two particles is presented when varying Γ (the markers correspond to the results of Deepwell et al. [16]). Qualitative results for two simulations ($\Gamma = 0.1$ and $\Gamma = 0.5$) at $t = 6$ and $t = 30$ are also presented. The particle Reynolds number (using the Stokes velocity scale) was set at $Re = 1/4$, Sc was fixed at 700, and the initial orientation angle ϕ was set at 67.5° . In panel (b), the simulation setup for oblate spheroids settling in-line is presented showcasing the subdomain decomposition and the background colour map illustrates the linear background density field. In panel (c), a schematic of the spheroidal axes are presented, where the polar radius of the spheroid is denoted as (a) , and the equatorial radius as (b) . The definitions of the aspect ratio ($\mathcal{AR} = a/b$) and the polar angle (θ) are also presented, where $\mathcal{AR} < 1$ is for an oblate spheroid, $\mathcal{AR} = 1$ is for a sphere, and $\mathcal{AR} > 1$ is for a prolate spheroid. In panel (d), a schematic of the initial separation distance between the leading and trailing particles (s_0) is presented, and a comparison of the average settling velocity V_z for a pair of oblate spheroidal particles with $\mathcal{AR} = 1/3$ with the numerical results of Ardekani et al. [41] is presented for $Ar = 80$ 94

5.2	Panel (a) shows the time history of the surface-to-surface separation distance for a settling pair of spherical particles in a linearly stratified fluid, for both the SBS and in-line configurations. For comparison, results are also shown for the corresponding cases in a homogeneous ambient. The non-dimensional parameters for the stratified cases were $Ar = 4.65$, $Fr = 6$ and $Sc = 700$. Panels (b) and (c) present qualitative results for the two configurations before the particles reach the bottom of the domain.	95
5.3	Time history of the settling velocity of an oblate spheroidal particle pair with $\mathcal{AR} = 1/3$, $Ar = 4.65$, $Fr = 8$, and $Sc = 700$, comparing simulations using the incompressible Navier-Stokes equations with the Boussinesq approximation and without the Boussinesq approximation. .	99
5.4	Panels (a) and (b) present the temporal evolution of the average settling velocity and the normalised distance between the particle surfaces for an oblate particle pair settling in a background fluid of different Fr . Panels (c) and (d) present the same results for a prolate particle pair. Panels (e) and (f) showcase the difference in peak velocities between the leading and trailing particles across different Fr for the oblate and prolate pairs, respectively.	100
5.5	Difference between the stratification and homogeneous drag coefficients for different Fr for an oblate and a prolate spheroidal pair, shown in (a) and (b), respectively. The dashed and solid lines correspond to the leading and trailing particles, respectively. In panels (c) and (d), the temporal evolution of the buoyancy (dashed), net (solid), and hydrodynamic (dash-dotted) forces are plotted for an oblate and prolate pair, respectively.	102
5.6	Panels (a) and (b) showcase the flow field for a pair of (a) oblate and (b) prolate particles settling in a homogeneous fluid, where the background colourmap depicts the z -velocity field. The background streamlines presented are in the stationary reference frame, and the streamlines are in the reference frame of the leading particle. Panels (c) and (d) showcase the time history of the particle and fluid kinetic energies, respectively. The particle and fluid kinetic energies are normalised by their respective masses (MU^2).	104

5.7	Results for the dynamic interaction between two settling oblate spheroids under different conditions. From left to right of every row, each panel showcases the flow field (right side) and streamlines (left side) in the reference frame of the leading particle. The left side of each panel also presents contours depicting the distortion of the pycnoclines, which are coloured such that the dark blue represents a heavier fluid. The difference in density between two adjacent pycnoclines is $\Delta\rho_f/\gamma D_{eq} = 1.14$. The colour map in the flow field illustrates the fluid velocity. Rows (a-b) correspond to $(Ar, \mathcal{AR}, Fr, s_0) = (4.65, 1/3, 8, 1), (4.65, 1/3, 8, 2)$, respectively.	106
5.8	This figure showcases the settling dynamics (a-b) when varying s_0 for both an oblate and prolate particle pair. The results showcase the normalised settling velocities and separation distances between the two spheroids.	107
5.9	This figure showcases the particle and fluid kinetic energies when varying the initial separation distance for an oblate (panels (a) and (c)) and prolate (panels (b) and (d)) particle pair.	108
5.10	Results for the dynamic interaction between two settling prolate spheroids under different conditions. From left to right of every row, each panel showcases the flow field (right side) and streamlines (left side) in the reference frame of the leading particle. The left side of each panel also presents contours depicting the distortion of the pycnoclines, which are coloured such that the dark blue showcases a heavier fluid. The difference in density between two adjacent pycnoclines is $\Delta\rho_f/\gamma D_{eq} = 1.14$. The colour map in the flow field illustrates the fluid velocity. Rows (a-b) correspond to $(Ar, \mathcal{AR}, Fr, s_0) = (4.65, 3, 8, 1), (4.65, 3, 8, 2)$, respectively.	110

5.11	Panel (a) of this figure shows the evolution of the asymmetric side escape of the trailing particle for an oblate spheroidal pair when $Fr = 4$. At $t = 700$, panel (b) showcases the baroclinic vorticity contribution and contours of the shear rate near the particle surface. In panel (c), the three-dimensional trajectories of the trailing and leading particles are depicted, and panel (d) showcases the temporal evolution of the polar angle θ for two different Fr for an oblate spheroidal pair. Note that the pentagram in panel (d) is for the simulation end time. Panel (e) shows the evolution of the torques acting on the leading and trailing particles when $Fr = 4$. Panels (f) and (g) showcase the settling dynamics when $Fr = 4$ and varying the aspect ratio.	111
5.12	Panels (a) and (b) showcase the asymmetric side escape of the trailing particle when $Fr = 4$ for two different aspect ratios of oblate spheroids. The aspect ratios are $\mathcal{AR} = 2/3$ and $\mathcal{AR} = 1/2$, respectively. Panels (c) and (d) showcase the side views of the settling trajectories of the particle pair when varying $\mathcal{AR}$ and $Fr = 4$. Panel (e) showcases the evolution of the trailing particle's velocity profile when varying $\mathcal{AR}$ against the normalised density.	113
5.13	This figure shows the comparison in the separation distance S and the flow field at $t = 350$ when $Sc = 7$ (dashed lines) and $Sc = 700$ (solid lines) for oblate and prolate particles when $Ar = 4.65$ and $Fr = 8$	115
5.14	This figure showcases the transient dynamics of an oblate and prolate spheroidal pair settling in a linearly stratified fluid with $Fr = 8$, $Sc = 700$, and $Ar = 4.65$ for a vertical distance of $z = 24$, and settling in a fluid with constant density after that for a distance of $z = 24$. Panels (a) and (b) present the z and x particle velocities, and panel (c) showcases the temporal evolution of the vertical position of the spheroidal pair. The dashed white line in panel (c) is at $z = 24D_{eq}$, which is at the transition from linearly stratified above the line to constant density below the line. In panel (d), qualitative results are presented for the two cases after the particles cross the linearly stratified region at $t = 1040$. . .	116
5.15	This figure shows the 3D trajectories of the leading and trailing particles when varying Ar and $\mathcal{AR}$. Here, $Fr = 8$, $Sc = 7$, and Ar is varied from 19 to 105.	118

5.16	This figure shows the time history of the particle interaction when $\mathcal{AR} = 1/3$, $Ar = 19$, $Fr = 8$ and $Sc = 7$	118
5.17	Numerical setups used for the simulations of a sparse cluster of spheres with the relevant definitions. Setup 1 and Setup 2 are referred to as S1 and S2 in the text, respectively.	121
5.18	Panel (a) shows the top view of the entire simulation using S1 for a sparse cluster of spherical particles with $3 \leq N_p \leq 6$, initialised at the apices of a regular polygon. In panel (b), a top view of the experimental observations of Jayaweera et al. [174] are presented for similar configurations.	121
5.19	Transverse cluster variance $\langle r_t^2 \rangle$ from the simulations using S1 for $N_p = 26$, shown as a log-log plot for varying (Fr, Sc) . After an initial quadratic growth, the homogeneous case exhibits a $t^{2/3}$ scaling, consistent with Subramanian and Koch [53].	122
5.20	Panel (a) shows the settling velocity V_z and the increment of the total mean-square cluster radius $\Delta \langle r^2 \rangle$ (about the instantaneous centroid) for S1 simulations with $N_p = 26$, for varying (Fr, Sc) . Panel (b) shows a top view of the cluster at the end of the simulation for the homogeneous case and for $(Fr, Sc) = (14, 700)$	125
5.21	Simulations performed using S1 with a resolution of $D_p/\Delta x \approx 16$ for varying Fr and $Sc = 700$ depicting the time history of the centre of mass of the cluster in the x and y directions.	126
5.22	Setup 2 (S2): quasi-planar cluster crossing a sharp density transition layer. The dashed line marks the interface position z_{int} , and the dotted lines denote the 95% transition thickness of the prescribed density profile. From left to right, the panels show the mean settling velocity V_z , the mean lateral speed V_l , and the transverse cluster variance $\langle r_t^2 \rangle$, plotted against $\Delta z = z_0 - z$ for $N_p = 10$. Row (a) varies the interface strength Γ (fixed $Sc = 7$, $Ar = 13.1$); row (b) varies Sc (fixed $\Gamma = 0.6$); row (c) varies the transition-layer thickness parameter H ; row (d) varies Ar . Unless otherwise stated, $Ar = 13.1$, $Sc = 7$, $H = 1$	128

6.1	(a) The three-dimensional Cartesian cubic domain with a size of $16R \times 16R \times 16R$, showing the subdomain decomposition and the initial problem setup; (b) the initial separation distance between the particle and the bubble is shown.	134
6.2	Validation of the numerical technique: Panels (a) and (b) show a comparison of our predictions with the experimental data of Kosior et al. [178] for a freely-rising bubble interacting with a solid wall; (a) compares the bubble deformation as a ratio of the horizontal over the vertical bubble axis, and (b) depicts the spatio-temporal evolution of the bubble-wall collision; (c) (i)-(iii) compare the results of a rising bubble shape with the experimental results of Bhaga and Weber [61]. The top panel shows the three-dimensional illustrations of the terminal bubble shapes, and the bottom panel illustrates a slice of the interface superposed on the experimental results of Bhaga and Weber [61]. The parameter values are $(Ga, Bo) = (2.316, 29), (3.094, 29),$ and $(4.935, 29)$ for panels (i), (ii), and (iii), respectively.	136
6.3	This figure showcases the experimental results of Pierson and Magnaudet [102, 103] for a spherical particle crossing an immiscible interface under different configurations. The plots showcase the performance of this numerical method compared to the experimental results in estimating the entrained fluid volume V_e and the particle velocity V_z . Qualitative results from the simulations are also provided.	139
6.4	The left hand side of the figure provides an illustration of the contact line numerical methodology between a bubble and a solid wall or solid particle. The plot showcases the temporal evolution of the south pole of the bubble as it adheres to a solid wall with negligible inertia. The contact angle for this case was $\theta_A = 102, \theta_R = 99$. A qualitative comparison with the experimental results of Basarova et al. [89] is provided at different time steps.	140

- 6.5 Spatio-temporal evolution of the rising bubble as it approaches the particle is shown in (a) and (b). The snapshots of the bubble contours are shown for $t = 1, 2, 3, 4$, and the particle is only shown at $t = 4$. In panel (a), a scale indicating the separation distance is provided between the bubble and the particle, indicating the bubble and the particle's initial centre positions at z_b^0 and z_p^0 , respectively. The non-dimensional parameters are (a) $Bo = 0.5, Ga = 10, Ar = 10$, (b) $Bo = 5, Ga = 10, Ar = 10$; panels (d), (e) and (f) show the change in energy of the system for three different Bo numbers and maintaining $Ga = 10$, and they are $Bo = 0.5$, $Bo = 2.0$, and $Bo = 5.0$, respectively. Here, E_m is the mechanical energy of the system, such that $\Delta E_m = \Delta E_p + E_k$. A new timescale is introduced here, t^* , which corresponds to the time for the reversal of kinetic energy due to the interaction. Panel (c) showcases the relative velocity of the bubble and the particle when varying Bo and Ga at t^* , and also showcases the difference in buoyancy force between the bubble and the particle when varying ζ_p 142
- 6.6 Temporal evolution of the aspect ratio, χ , and the distance between the bottoms of the bubble and particle, S , shown in (a) and (b), respectively, for $Bo = 0.5$, $Bo = 2.0$, and $Bo = 5$, with $Ga = 10$, and $\zeta_p = 1$. Panel (c) showcases the minimum aspect ratio when varying Bo and maintaining $Ga = 10$, while also plotting the change in interfacial surface area at that timestep ($t_{\chi_{min}}$). The film thickness profile is presented for these cases at $t_{\chi_{min}}$ in panel (d), and the temporal evolution of the dimple radius R_D is presented in panel (e). 143
- 6.7 Spatio-temporal evolution of the bubble-particle interaction dynamics shown for the same parameters used to generate Fig. 6.5; the rows are associated with $Bo = 0.5$, $Bo = 2.0$, and $Bo = 5$, from top to bottom. The contours on the left part of the figures in the panels show the logarithm of the viscous dissipation function $\log_{10} \xi$ in the fluid, and the contours on the right show the velocity magnitude in the fluid V . The bubble is shown with glyphs of the velocity to illustrate the relative motion of the bubble at different time-steps. 146

- 6.8 This figure showcases the film thickness and the bubble shape as it approaches the particle when $Ga = 10$, $\zeta_p = 1$, and $Bo = 0.5$ in panels (a) and (b). In panels (c) and (d), the temporal evolution of the kinetic energy and particle velocity is presented for two cases, and they are when $\Omega = 1$, which is the base case, and when $\Omega = 2$. In panels (e) and (f), the film thickness profile and the bubble shape at different time steps during the interaction for $\Omega = 2$ are presented. 147
- 6.9 The spatio-temporal evolution of the bubble-particle interaction dynamics is shown in (a) for $Ga = 10$, $Bo = 2$ and $\zeta_p = 1$, where the contours depict the velocity magnitude. Panel (b) shows the spatio-temporal evolution of the interaction dynamics when $Ga = 10$, $Bo = 5$ and $\zeta_p = 1$. The timesteps presented are relative to t^* , such that $t - t^*$ varies from 2.5 to 7.0. When $Bo = 2$ and $t - t^* = 7$, a top view of the interaction between the bubble and the particle is presented to showcase that no contact is found between them. In panels (c) and (d), the normalised energy budget $\tilde{E}/\tilde{E}_0$ is presented for $Bo = 2$ and $Bo = 5$, respectively, where $\tilde{E}_0 = E_{p0}^{particle} + E_{s0}$ 148
- 6.10 Panels (a) and (b) show the temporal evolution of the minimum gap thickness $h(t)$ for different Bo when $Ga = 10$ and $\zeta_p = 1$. Two different scalings are also provided, such that $h \sim (t - t^*/t_d)^{-\alpha}$ where α here is either $4/5$ or $1/2$ 149
- 6.11 In panels (a), (b) and (c), the particle settling velocity, total kinetic energy, and the change in particle potential energy are presented, respectively. These results correspond to when $Ga = 20$, $Bo = 0.5$ and varying ζ_p . Temporal evolution of the minimum gap thickness $h(t)$ is shown in (d) for $\zeta_p = 1$, $Ga = 20$, and $Bo = [0.5 - 5]$; an enlarged view of the plot in (d) is shown in panel (f), for $Bo = 0.5$ and $Bo = 1$ as at these Bo numbers, the bubble did not rupture. A scaling for the film drainage is provided such that $h \sim ((t - t^*)/t_d)^{-4/5}$. Panel (e) showcases the film thickness profile at $t_{\chi_{min}}$ when varying Bo and maintaining $Ga = 20$ and $\zeta_p = 1$ 151

- 6.12 This figure showcases the dynamics of the interaction after the formation of the contact line, when $Ga = 10$, $Bo = 0.5$, and $\zeta_p = 1$. In panel (a), the particle's vertical velocity is presented for different particle wettability parameters, which correspond to a base case with $\theta_e = 105^\circ$, and two additional cases with $\theta_e = 55$, and $\theta_e = 125$. The figures on the right-hand side correspond to $t - t^*$ from 8 to 11 for the base case and $t - t^*$ from 5 to 7 when $\theta_e = 55^\circ$. Panel (b) showcases the aspect ratio χ for the three different cases. Lastly, panel (c) showcases the temporal evolution of the radius of the contact line R_{TPC} when varying θ_e and Ω . Note that the x -axis is scaled with the contact line time t_{TPC} 152
- 6.13 Spatio-temporal evolution of off-centre bubble-particle interaction dynamics with $Ar = 10$, $Ga = 10$, and an initial bubble location offset of $\delta = 1$. The results shown in the top and bottom two rows were generated with $Bo = 0.5$ and $Bo = 5$, respectively. The contours are of the logarithm of the viscous dissipation function $\log_{10} \xi$ in the fluid. The bubble is shown with glyphs of the velocity to illustrate the relative motion of the bubble at different time-steps. The snapshots are shown between $t = 2.5$ and $t = 6$ in time-increments of $\Delta t = 0.5$ 156
- 6.14 Temporal evolution of the total kinetic energy, and the change in bubble surface area are shown in (a)-(b), respectively, for off-centre bubble-particle interactions with $(Bo, Ga, Ar, \delta) = (0.5, 10, 10, 1)$ and $(5, 10, 10, 1)$. Panels (c) and (d) show the temporal evolution of the settling velocity, and the x -component of the particle velocity, respectively. In panels (e) and (f), the side view of the particle trajectory with respect to the x -axis and the y -axis are presented, respectively. 157

6.15	The top two panels (a) and (b) show the total kinetic energy of the system and the distance between the particle south pole and the bubble south pole (S), at two different resolutions for $Ga = 10$, $Bo = 0.5$, and $\zeta_p = 1$, respectively. Panel (c) shows the temporal evolution of the total kinetic energy when increasing the domain size for the same case. It can be seen that increasing the domain size leads to no difference in the results. Panel (d) shows the total kinetic energy for different mesh sizes for $Ga = 10$, $Bo = 5.0$, and $\zeta_p = 1$, up to a resolution of $\Delta x/R = 1/64$. The results show that the domain size and mesh resolution utilised in this work is sufficient to capture the dynamics of the interaction between the bubble and the particle.	160
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List of Tables

2.1	Dimensionless momentum (δ_m) and diffusive (δ_ρ) boundary layer thickness estimates from the literature [11, 27].	20
4.1	Simulation setup utilised for the homogeneous fluid benchmark cases. . . .	64
5.1	Simulation setup utilised for setups S1 and S2.	120

Notation

All symbols and abbreviations used in this thesis are defined at their first occurrence and are summarised in the list below. For the reader's convenience, the definitions of certain key symbols and abbreviations introduced in earlier chapters are occasionally reiterated in subsequent chapters.

Abbreviations

AMR Adaptive mesh refinement

CFD Computational fluid dynamics

CFL Courant-Friedrichs-Lewy

DKT Drafting-kissing-tumbling

DNS Direct numerical simulations

ENO Essentially non-oscillatory

FSI Fluid-structure interaction

GMRES Generalised Minimal Residual

GNBC Generalised Navier Boundary Condition

HPC High-performance computing

IBM Immersed boundary method

LCRM Level Contour Reconstruction Method

LHS Left-hand side

MAC Marker-and-Cell

MPI	Message passing interface
PLIC	Piece-wise linear interface calculation
RHS	Right-hand side
RMSE	Root mean squared error
SBS	Side-by-side
SOR	Successive over-relaxation
VOF	Volume of fluid
2-D, 3-D	Two- and three-dimensional, respectively

Greek letters and operators

α	Scaling exponent, growth exponent, or empirical drag exponent
β	Density ratio in bubble–liquid systems, or thermal expansion coefficient where specified
Γ	Stratification strength in sharp density transition layers, or circulation
γ	Surface tension, or background density gradient
δ	Dirac delta distribution, or horizontal offset in off-centre bubble–particle interactions
Δ	Change in a quantity, difference operator, or grid spacing when used with x , y , or z
Δt	Time step
ϵ	Dimensionless gap/separation parameter in lubrication corrections
η	Viscous dissipation contribution when used in E_η
θ	Particle inclination angle or contact angle, depending on context
$\theta_A, \theta_R, \theta_e$	Advancing, receding, and equilibrium contact angles, respectively
κ	Molecular diffusivity of the stratifying agent, or curvature where specified
λ	Viscosity ratio, or lubrication correction function where specified
μ	Dynamic viscosity
ν	Kinematic viscosity
ρ	Density
ρ_0	Reference density
ρ_f, ρ_p	Fluid and particle densities, respectively

ρ_b, ρ_l	Bubble and liquid densities, respectively
$\hat{\rho}$	Positive relative density contrast used in Chapter 4, $(\rho_{f,0} - \rho_p)/\rho_{f,0}$
$\bar{\rho}$	Particle-to-fluid density ratio
$\bar{\mu}$	Phase viscosity ratio
$\tau, \boldsymbol{\tau}$	Stress or stress tensor
ϕ	Generic signed-distance function, or particle-pair orientation angle where specified
ϕ_f, ϕ_s	Signed-distance functions for the fluid/fluid and solid/fluid interfaces, respectively
Φ	Eulerian field obtained by spreading interfacial source terms
ψ	Generic interfacial source term
$\omega, \boldsymbol{\omega}$	Angular velocity or vorticity, depending on context
ζ_p	Relative solid–fluid density contrast, $(\rho_p - \rho_l)/\rho_l$
$\Omega(z)$	Local particle-to-fluid density ratio in Chapter 5, $\rho_p/\rho_f(z)$
Ω	Bubble-to-particle radius ratio in Chapter 6, R_b/R_p
∇	Nabla operator
∇_h	Spatially discrete Nabla operator
∇_s	Surface gradient operator

Dimensionless numbers

Ar	Archimedes number
Bo	Bond number
Ca	Capillary number
Fr	Froude number
Ga	Galilei number
I, I^*	Dimensionless moment of inertia
Oh	Ohnesorge number
Pe	Peclet number
Pr	Prandtl number
Re	Reynolds number
Ri	Richardson number
Sc	Schmidt number
St	Strouhal number
St	Stokes number
$\chi, \mathcal{AR}$	Aspect ratio

Roman symbols

a, b	Polar and equatorial spheroid radii, respectively
A, A_0	Interfacial area and initial interfacial area
C_D	Drag coefficient
C_D^H	Drag coefficient in a homogeneous fluid
C_D^S	Drag coefficient in a stratified fluid
ΔC_D	Stratification-induced drag enhancement
d	Diameter of the central perforation in annular discs
D_D	Disc diameter
D_p	Particle diameter
D_{eq}	Volume-equivalent particle diameter
$\mathbf{e}_z$	Unit vector in the vertical direction
E_k	Kinetic energy
E_p	Potential energy
E_s	Surface energy
E_η	Viscous dissipation energy
E_m	Mechanical energy
F_B	Buoyancy force
F_H	Hydrodynamic force
F_T	Total force
$\mathbf{F}_{FSI}$	Fluid–solid interaction forcing term
g	Gravitational acceleration
$h(t)$	Minimum bubble–particle gap thickness
$h_0(t)$	Centreline bubble–particle gap thickness
H	Density-transition-layer thickness parameter
$\mathcal{H}$	Generic Heaviside/indicator function
$\mathcal{H}_f$	Fluid-phase Heaviside function
$\mathcal{H}_s$	Solid Heaviside function
L	Characteristic length scale
L_x, L_y, L_z	Computational domain dimensions
m_p	Particle mass
N	Brunt–Vaisala frequency
N_p	Number of particles
p	Pressure
R	Characteristic radius
R_b, R_p	Bubble and particle radii, respectively
R_c	Cluster radius

R_D	Dimple radius
R_{eq}	Equivalent spherical particle radius
R_{TPC}	Three-phase contact-line radius
$\langle r_t^2 \rangle$	Transverse cluster variance
s_0	Initial surface-to-surface particle separation
S	Distance between the particle south pole and bubble south pole
t	Time
t^*	Time associated with reversal of kinetic energy during bubble-particle interaction
t_d	Film-drainage time scale
t_{TPC}	Contact-line time scale
U	Characteristic velocity
U_s	Stokes settling velocity
$\mathbf{u}$	Fluid velocity field
$\mathbf{u}_p$	Particle translational velocity
V	Velocity magnitude
V_x, V_y, V_z	Cartesian velocity components
V_l	Lateral particle speed, $\sqrt{V_x^2 + V_y^2}$
V_e	Entrained volume
$\mathcal{V}$	Particle volume or solid volume
$\mathbf{x}$	Position vector
$\mathbf{x}_f$	Interfacial marker position
x, y, z	Cartesian coordinates
x_{cm}, y_{cm}	Cluster centroid coordinates in the horizontal directions
z_0	Initial vertical position
z_{int}	Initial interface height
Δz	Vertical distance travelled relative to the initial position

General rules

- Tildes ($\sim$) denote dimensionless variables.
- Unless otherwise stated, subscripts f , p , s , b , and l denote fluid, particle, solid, bubble, and liquid phases, respectively. Subscript 0 denotes an initial or reference value.
- Superscripts H and S on drag coefficients denote homogeneous-fluid and stratified-fluid values, respectively.

- In this thesis, the Prandtl (Pr) and Schmidt (Sc) numbers are used interchangeably to denote the ratio of momentum diffusivity to scalar diffusivity, with Pr usually associated with thermal stratification and Sc with solutal stratification.

Chapter 1

Introduction

Contents

1.1	Motivation and scope	2
1.2	Thesis outline	6

1.1 Motivation and scope

Marine debris is a major environmental issue in the modern world. In 2015, there were approximately 5 trillion pieces of plastic waste in the ocean [1], posing risks to marine life and potentially to human health. Plastic debris can be ingested by marine organisms and can also contribute to the release and transport of chemical contaminants in the marine environment, highlighting the threat that plastic pollution poses to marine ecosystems. Moreover, plastics have been detected throughout the food chain, underscoring their potential implications for human exposure and health [2]. A large portion of this debris ultimately disintegrates into smaller particles covering a wide spectrum of sizes. Microplastics are typically defined as plastic particles with sizes from 1 μm to 5 mm [3]. Particles larger than this range are commonly categorised as mesoplastics (5–20 mm) and macroplastics (> 20 mm). Nanoplastics (often $< 1 \mu\text{m}$) are also receiving growing attention; however, standardised and reliable approaches for their detection and characterisation in environmental samples remain under development [3]. Although macroplastics dominate the total plastic mass in the ocean, microplastics are believed to be the most numerous size class [4]. These microplastics arise both from primary inputs to the ocean and from the secondary fragmentation of larger debris, producing diverse morphologies such as microfibers or thin planar fragments.

Microplastic transport is also shaped by strong variability in the underlying material properties. At the ocean surface, polyethylene and polypropylene for instance are frequently reported among the dominant polymer types [3]. These materials tend to be relatively buoyant in seawater [5], whereas other plastics are more prone to submergence because they are typically heavier than seawater [5]. As a result, many particles fall into a regime where their buoyancy is weak, so modest changes in their properties or in local fluid conditions can substantially alter whether they reside near the surface or are transported downwards.

Crucially, these properties are not fixed. Apparent buoyancy can shift over time as biofouling and biological growth accumulate on the particle [6], and as weathering modifies the material properties [7, 8]. In addition, microplastic particles may not be uniform, as shown in panel (b) of Fig. 1.1, so different areas can respond differently to the flow conditions. Surface chemistry evolves as well: plastics that are initially strongly hydrophobic can become more wettable through aging and photochemical alteration [8]. This progression matters for bubble scavenging (illustrated in panel (a) of Fig. 1.1), in which rising bubbles capture suspended particles by attachment at the air/water interface and carry them upward. Bubble-driven transport can therefore elevate near-surface concentrations,

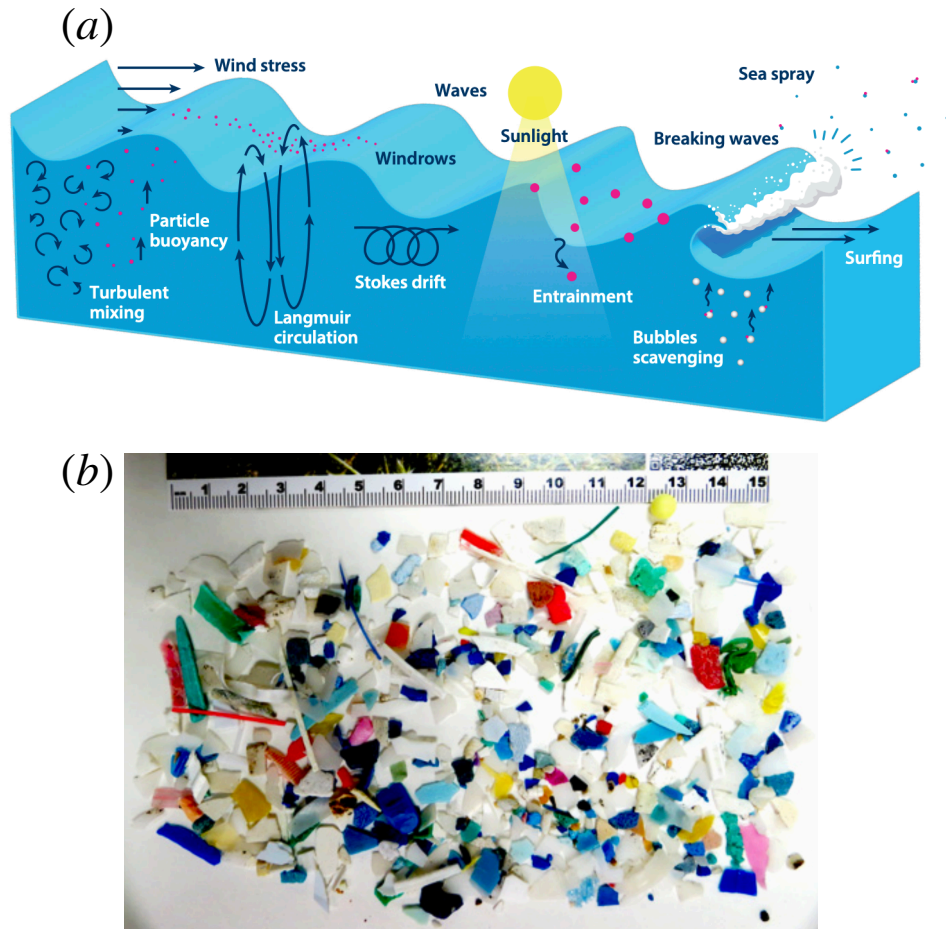


Figure 1.1: Panel (a) shows a schematic of relevant processes near the ocean surface, adapted from DiBenedetto [3]. Panel (b) shows the plethora of different shapes of plastics found in the ocean, adopted from Sutherland et al. [9].

while subsequent bubble bursting can return particles to the near-surface layer and potentially inject them into sea-spray aerosols. The effectiveness of this pathway depends sensitively on particle morphology and surface chemistry, along with particle size.

Many of the mechanisms that control where plastic ultimately ends up in the ocean remain unresolved, especially below the surface. Although large scale studies that merge ocean circulation models with surface measurements have successfully highlighted persistent convergence zones, including subtropical gyres where buoyant debris commonly accumulates, these advances do not yet translate into a comparable understanding of subsurface pathways. Processes such as downward transport, coastline retention, and continued breakdown into smaller pieces are still not well constrained, even though they are central to balancing the marine plastic budget. Progress is hindered by the breadth of scales involved. Plastic spans an enormous range of particle sizes, and it is exposed to forcing that ranges from basin scale currents to fine scale turbulent motions. In addition to this wide span of physical processes, microplastic behavior is intertwined with chemical

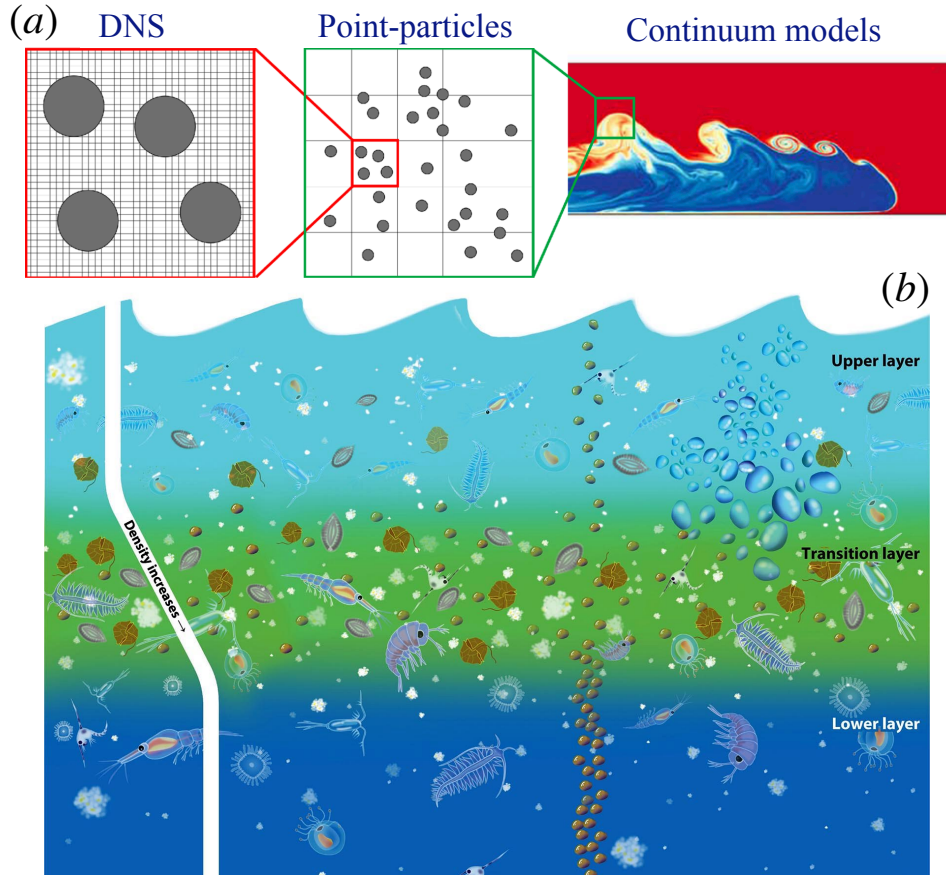


Figure 1.2: Panel (a) presents an illustration of the different scales governing the transport of microplastics in the ocean, adopted from Vowinckel [10]. Panel (b) illustrates the inherent density-stratification in the ocean, adopted from More and Ardekani [11].

transformations and biological interactions, making reliable fate and transport predictions an inherently multidisciplinary problem.

The abundance of plastic debris in the ocean therefore serves as a primary motivation to carry out this research. In this project, the focus is broadly on the transport of particles in inhomogeneous fluids, with the goal of developing a particle-scale understanding that can ultimately inform predictive models relevant to marine plastic pollution.

Particles settling in stratified fluids are encountered across a variety of settings, including engineering applications and oceanography [12]. In oceanography, plankton, marine snow, and plastic debris often move through fluids characterised by strong density gradients arising from temperature-driven stratification (thermoclines) and salinity-driven stratification (haloclines). The density-stratification in the ocean is illustrated in panel (b) of Fig. 1.2. As the surrounding fluid density increases with depth, settling (or rising) rates can change dramatically, making the study of particle motion in such environments essential for understanding and predicting transport pathways. These pathways are rel-

evant to applications including the rise times of oil droplets following spills [13] and the drift of Lagrangian buoys [14]. More broadly, understanding how oceanic inhomogeneity shapes particle transport can improve our understanding of marine pollution pathways and biogenic mixing.

When considering particles such as microplastics, marine snow, planktonic aggregates, and oil droplets in natural waters, vertical transport is often controlled by relatively thin stratified layers embedded within much deeper water columns. These include seasonal thermoclines and metalimnia in lakes, estuarine haloclines, coastal pycnoclines, and the base of the ocean mixed layer. The relevant vertical gradients may extend over centimetres to metres, whereas the particles interacting with them typically span micron to millimetre scales. Such interfaces can alter particle residence times and produce local accumulation; for example, MacIntyre et al. [15] reported enhanced marine snow concentrations at density discontinuities in the water column. This provides a direct environmental context for idealised simulations in which the particle-scale response to density gradients is isolated from the larger-scale circulation. These field observations also provide useful estimates for the relevant particle-scale non-dimensional parameters. Drawing on the marine-snow measurements of MacIntyre et al. [15], Deepwell et al. [16] noted that particles settling in the ocean can correspond to Reynolds numbers in the range $Re \simeq 0.2\text{--}23$ and Froude numbers in the range $Fr \simeq 5\text{--}70$, where Re is based on the particle size and settling velocity and Fr compares the settling time scale with the local buoyancy time scale. These ranges indicate that environmentally relevant particles may experience both viscous and inertial effects at the particle scale, while still being strongly influenced by stable density gradients near interfaces. The simulations considered in this thesis therefore target idealised but environmentally motivated regimes in which finite particle inertia and stratification can jointly modify settling, rising, and interaction dynamics.

Owing to the wide range of relevant length and time scales in the realm of geophysical fluid dynamics, the development of reliable numerical models across scales has been an active research area. Processes can be segregated by scale, as illustrated in panel (a) of Fig. 1.2, where each regime calls for a different modeling approach. At the microscale, particle-resolved Direct Numerical Simulations (DNS) compute the motion in every cell by solving the governing flow equations alongside the Newton–Euler equations for particle dynamics, accounting for relevant forces and fully resolving the particle/fluid interaction. At the meso-scale, the point-particle concept represents potentially millions of particles as subgrid-scale entities whose dynamics are governed by empirical or semi-empirical closures; particles are simplified as mass points whose effects are modeled rather than resolved. At the macroscale, length scales can extend to kilometers and beyond, and

modeling typically relies on continuum formulations using coupled transport equations in which individual grains are not resolved.

These approaches differ in fidelity and computational cost, with DNS generally being the most expensive [10]. Nevertheless, microscale studies remain highly valuable because they can identify mechanisms that influence behaviour across scales and provide physically grounded insight that improves the accuracy of larger-scale models, particularly in regimes where small-scale processes such as vertical transport and stratification-mediated dynamics control the ultimate fate of microplastics.

1.2 Thesis outline

This thesis seeks to build upon the current fundamental understanding of particle dynamics in environments representative of those encountered by microplastics, with particular emphasis on density-stratification, particle geometry, particle-particle interactions, and multiphase effects such as bubble-particle interactions. Furthermore, this thesis is based on particle-scale direct numerical simulations (DNS) of freely moving particles and bubbles in otherwise quiescent fluids, resolving the flow around individual particles and their interactions with density-stratification and deformable interfaces. The remainder of the thesis is structured as follows. Chapter 2 presents a brief review of the relevant literature. Chapter 3 describes the methodology and numerical framework utilised in this thesis. Chapter 4 investigates the role of particle geometry in the rising dynamics of particles within density-stratified fluids. Chapter 5 examines the influence of particle-particle interactions in density-stratified fluids. Chapter 6 focuses on bubble-particle interactions. Finally, Chapter 7 summarises the main findings and outlines directions for future work.

Chapter 2

Literature review

Contents

2.1	Governing physics	8
2.2	Particle dynamics in homogeneous fluids	11
2.3	Boussinesq approximation	16
2.4	Particle dynamics in density-stratified fluids	18
2.4.1	Flow field and transient behaviour	19
2.4.2	Particle shape and porosity	23
2.4.3	Particle-particle interactions	25
2.4.4	Drag Enhancement	29
2.5	Particles, drops and bubbles	30
2.6	Summary and remarks	34

2.1 Governing physics

As discussed in Chapter 1, particulate flow in the ocean can be associated with the viscous or inertial regime, depending on the size of the particles. Let us consider for instance the flow past a rigid (non-deformable) particle of arbitrary shape, as shown in panel (a) of Fig. 2.1. For incompressible flow of a Newtonian fluid, the motion is governed by the equations of mass and momentum conservation, which may be written as:

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

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right) = -\nabla p^a + \mu \nabla^2 \mathbf{u} + \mathbf{F}, \quad (2.2)$$

where $\mathbf{u}$ is the fluid velocity, ρ is the density, p^a is the absolute pressure, μ is the constant dynamic viscosity, and $\mathbf{F}$ is the external body force per unit volume (such as gravity). The first and second terms on the right hand side of Eq. 2.2 may be written in terms of the ‘absolute’ stress tensor $\nabla \cdot \boldsymbol{\sigma}^a$ where $\boldsymbol{\sigma}^a = -p^a \mathbf{I} + \mu (\nabla \mathbf{u} + \nabla \mathbf{u}^T)$. A modified stress tensor will be defined later.

Prior to discussing the equations governing particle motion, we start by considering the boundary conditions that arise on the particle surface due to the ambient fluid motion. Under the no-slip condition, the velocity of the fluid at the particle surface matches the velocity of the particle surface at that point. At the particle surface, this may be written as:

$$\mathbf{u}(\mathbf{x}) = \mathbf{u}_p + \boldsymbol{\omega}_p \times (\mathbf{x} - \mathbf{x}_0), \quad (2.3)$$

where $\mathbf{u}_p$ and $\boldsymbol{\omega}_p$ are the translational and rotational particle velocities, respectively. The three-dimensional spatial coordinate is taken as $\mathbf{x}$, and the particle centre is denoted as $\mathbf{x}_0$. Considering multiple particles as illustrated in panel (a) of Fig. 2.1 means that the appropriate boundary condition must be imposed on the surface of every particle.

Let us now consider the role of the body force term $\mathbf{F}$. The usual external force due to gravity may be written as $\mathbf{F} = \rho \mathbf{g}$, where $\mathbf{g}$ is the gravitational acceleration. If the external force is conservative, its gradient can be absorbed into a modified pressure field defined as $p = p^a - \rho \mathbf{g} \cdot \mathbf{x}$. This modified pressure field is what we call the dynamic pressure. Furthermore, the fluid surrounding an immersed particle exerts a force on the particle surface. Considering an immersed particle in a liquid subjected to a uniform gravitational field, the total force on the particle surface is dictated by the integral of the traction vector $\boldsymbol{\sigma}^a \cdot \mathbf{n}$, where $\mathbf{n}$ is the outward facing normal from the surface of the

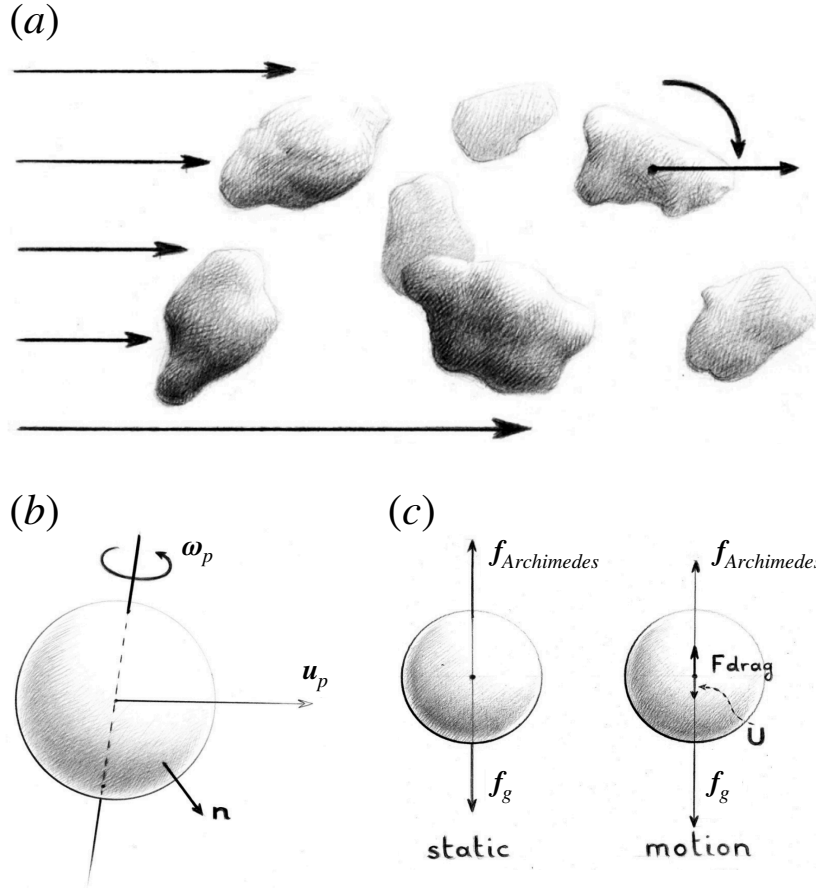


Figure 2.1: Panel (a) shows many particles of arbitrary shape in a background flow. Panel (b) depicts a spherical particle with translational velocity $\mathbf{u}_p$ and angular velocity $\boldsymbol{\omega}_p$, and an outward-pointing normal $\mathbf{n}$. Panel (c) illustrates the force balance for a stationary spherical particle and for a spherical particle in motion. The panels are adapted from Guazzelli and Morris [17].

particle (see panel (b) of Fig. 2.1):

$$\mathbf{f} = \int_S \boldsymbol{\sigma}^a \cdot \mathbf{n} \, dS. \quad (2.4)$$

If we consider the particle to have a uniform density ρ_p and is spherical in shape with a radius of a , the gravitational force acting on the body would be $\mathbf{f}_g = 4/3 \, \pi a^3 \rho_p \mathbf{g}$. For a neutrally buoyant static particle ($\rho_p = \rho$), the gravity force $\mathbf{f}_g$ is balanced by the fluid forces around the particle surface, such that $\mathbf{f} = -\mathbf{f}_g$. This is generally called Archimedes' principle, and an illustration is included in panel (c) of Fig. 2.1. Under these conditions, particle motion is a result of a difference between the particle density ρ_p and the ambient fluid density ρ , as seen in panel (c). If the particle density is slightly larger than that of the ambient fluid, the particle will sink. However, if the particle density is lower than the fluid density, the fluid force on the surface of the particle exceeds the

gravitational force, causing the particle to rise.

The importance of separation between the absolute and modified pressure fields is to determine the resulting hydrodynamic force acting on the particle surface in the case of its motion. The drag force is the component of the hydrodynamic force that acts opposite to the direction of motion of the particles, as seen in the illustration provided in panel (c). To quantify the hydrodynamic force acting on the particle surface, a dynamic stress is defined as $\boldsymbol{\sigma} = \boldsymbol{\sigma}^a + \rho(\mathbf{g} \cdot \mathbf{x})\mathbf{I}$, where $\mathbf{I}$ is the identity matrix. The hydrodynamic force may then be defined as:

$$\mathbf{f}_H = \int_S \boldsymbol{\sigma} \cdot \mathbf{n} dS. \quad (2.5)$$

Under steady state conditions, $\mathbf{f}_H$ is instantaneously balanced by the excess weight of the particle, such that:

$$\mathbf{f}_H = -\frac{4}{3}\pi a^3 \Delta\rho \mathbf{g}, \quad (2.6)$$

where $\Delta\rho$ is the difference between the particle and ambient fluid density. Furthermore, the hydrodynamic torque about the reference point $\mathbf{x}_0$ is obtained by integrating the moment of the surface traction over the particle surface,

$$\mathbf{T}_H = \int_S (\mathbf{x} - \mathbf{x}_0) \times (\boldsymbol{\sigma} \cdot \mathbf{n}) dS, \quad (2.7)$$

where $(\mathbf{x} - \mathbf{x}_0)$ is the lever arm relative to $\mathbf{x}_0$, and will be defined as $\mathbf{r}$.

Having defined the hydrodynamic force and torque on the particle through Eqs. (2.5) and (2.7), the translational and rotational motion of a rigid particle follow from the Newton-Euler equations. Let the particle have volume $\mathcal{V}$ and density ρ_p , so that its mass (m_p) is

$$m_p = \rho_p \mathcal{V}. \quad (2.8)$$

As the stress tensor $\boldsymbol{\sigma}$ was defined by removing the hydrostatic contribution (i.e. using $p = p^a - \rho \mathbf{g} \cdot \mathbf{x}$), the gravitational forcing enters the particle equation through the *excess weight* $(\rho_p - \rho)\mathcal{V}\mathbf{g}$. The translational equation of motion is therefore:

$$m_p \frac{d\mathbf{u}_p}{dt} = \mathbf{f}_H + (\rho_p - \rho) \mathcal{V} \mathbf{g} + \mathbf{f}_{\text{ext}}, \quad (2.9)$$

where $\mathbf{f}_{\text{ext}}$ denotes any additional external forces, including contact forces.

The rotational dynamics about $\mathbf{x}_0$ are governed by the angular momentum balance. Let $\mathbf{I}_p$ denote the particle inertia tensor about $\mathbf{x}_0$. The Newton-Euler equation takes the

standard form

$$\frac{d(\mathbf{I}_p \boldsymbol{\omega}_p)}{dt} = \mathbf{T}_H + \mathbf{T}_{\text{ext}}, \quad (2.10)$$

where $\mathbf{I}_p$ denotes the moment of inertia tensor and $\mathbf{T}_{\text{ext}}$ represents any external torques (including those resulting from particle-particle contact). The moment of inertia of an arbitrarily shaped particle varies with the particle orientation, and is therefore kept in the time derivative. Eqs. 2.9 and 2.10 are the underlying governing equations that describe particulate transport, modeled in this thesis.

2.2 Particle dynamics in homogeneous fluids

In this section, we provide a generic overview of the different regimes observed for rising and settling bodies in homogeneous fluids. Here, a *homogeneous* fluid refers to a fluid without ambient density stratification.

It is useful to begin by defining the main non-dimensional parameters governing the flow dynamics. If the Navier-Stokes equations (2.2) are non-dimensionalised using appropriate characteristic scales (a characteristic length L , velocity U , and kinematic viscosity ν), the Reynolds number is defined as

$$Re = \frac{UL}{\nu}, \quad (2.11)$$

which represents the ratio of inertial to viscous forces in the flow. Typically, for freely rising or settling bodies, the characteristic velocity used to define the Reynolds number is the body's terminal velocity, which is attained after an initial transient associated with the object's acceleration from rest. When performing experiments and simulations, this terminal velocity is unknown *a priori*. Therefore, it is useful to define a gravitational velocity scale, which leads to the definition of the Archimedes (or Galilei) number. This

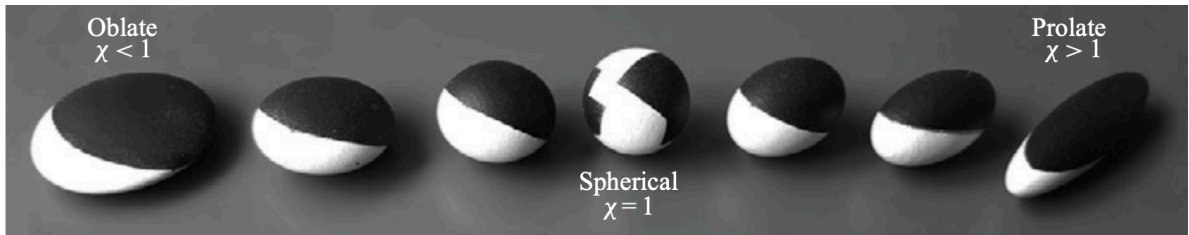


Figure 2.2: Shape of spheroids when varying the aspect ratio χ . Figure adapted from Will et al. [18].

gravitational velocity scale is typically a function of the density ratio between the particle and the ambient fluid ($\bar{\rho} = \rho_p/\rho_f$), such that $U_g = \sqrt{g|\bar{\rho} - 1|L}$. The Archimedes number may then be defined as:

$$Ar = \frac{U_g L}{\nu}. \quad (2.12)$$

In simulations and experiments of flow past a static body, the characteristic velocity scale is the imposed flow velocity; therefore, this distinction between the Reynolds number and the Archimedes number is not required.

Additionally, the shape of the particles needs to be characterised, since it can strongly influence drag, wake structure, and the onset of path instabilities. For non-spherical bodies, this is typically done by introducing one or more geometric parameters, such as an aspect ratio χ ($\chi = a/b$ for a spheroid with semi-axes a and b , or $\chi = D/L$ for a cylinder of length L and diameter D). For more general shapes, a convenient single-parameter measure is the sphericity, often defined as $\Psi = A_s/A_p$, where A_s is the surface area of a sphere having the same volume as the particle and A_p is the particle surface area. In practice, it is also common to define a reference length scale based on the particle volume (such as an equivalent-volume diameter) so that comparisons across different shapes can be made consistently.

In this thesis, we limit our investigation to particles of three different shapes, namely spheres, discs, and spheroids. Therefore, the aspect ratio is sufficient to characterise the particle shape. In the chapters concerning discs and spheroids, the aspect ratio is defined as either χ for discs or $\mathcal{AR}$ for spheroids, so that the distinction is clear. For the remainder of this chapter, we adopt the notation χ to denote the aspect ratio. Fig. 2.2 shows the difference in spheroidal shapes when varying the aspect ratio χ . When $\chi < 1$, the shape of the particle corresponds to an oblate spheroid, while for $\chi > 1$, the particle corresponds to a prolate spheroid. The limiting case $\chi = 1$ recovers a sphere. In the extreme oblate limit $\chi \ll 1$, the particle becomes disc-like, while in the extreme prolate limit $\chi \gg 1$ it becomes rod-like. The spheroidal spectrum therefore provides a good modelling approximation for the range of microplastic shapes introduced in Chapter 1.

When rotational motion is permitted, the particle's response to hydrodynamic torques depends on its rotational inertia. It is thus useful to define the mass moment of inertia with respect to the principal axes. For a disc-shaped particle, these correspond to the symmetry axis normal to the disc and an in-plane axis through the centre of mass. For rising and settling discs in a broadside-on orientation (meaning the projected area normal to the direction of motion is maximised), the relevant rotation is about an in-plane axis through the centre of mass. For a homogeneous circular disc of diameter D and thickness

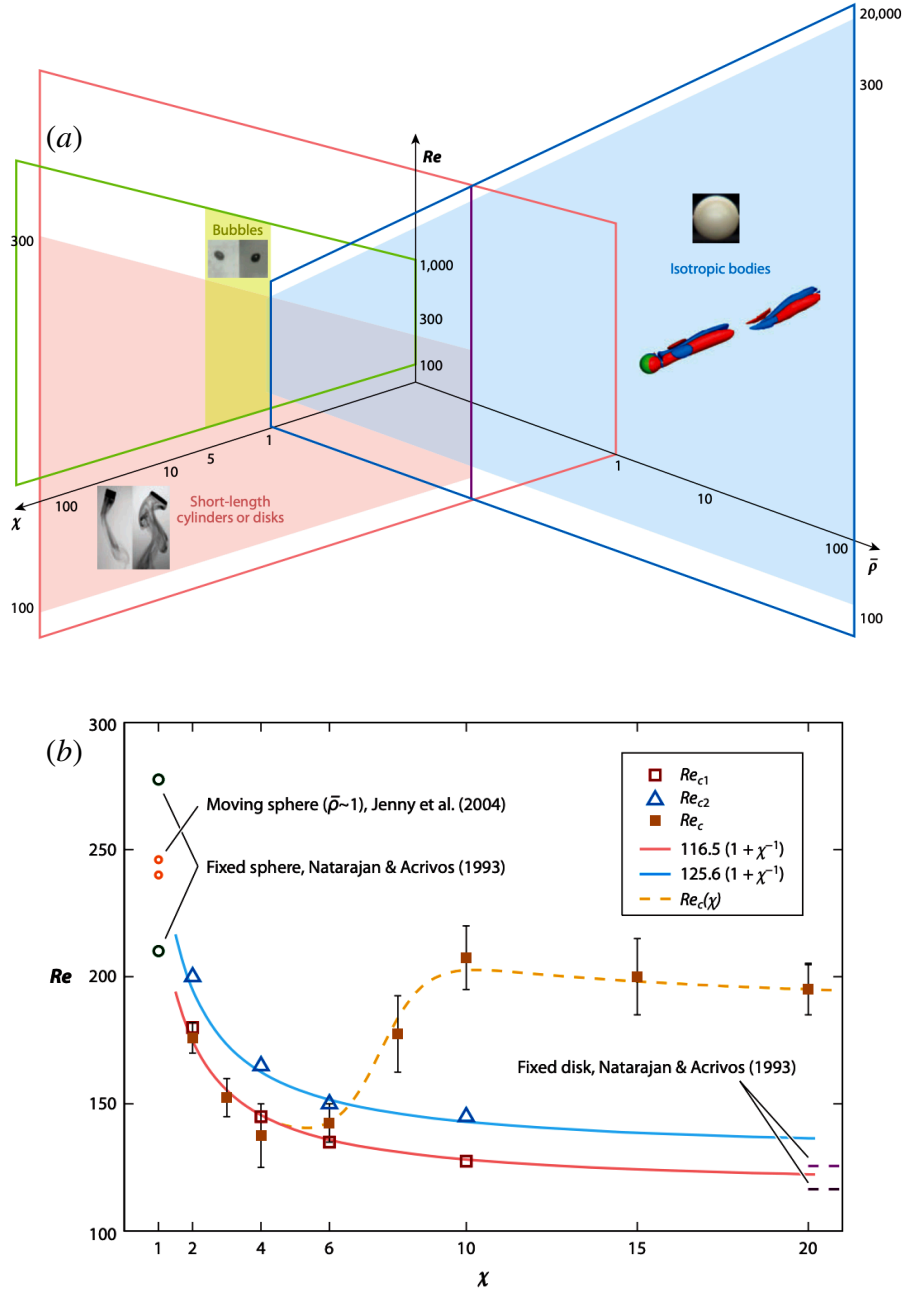


Figure 2.3: Panel (a) shows some of the investigated parameter ranges in a three-dimensional parameter space $(\bar{\rho}, Re, \chi)$, and panel (b) presents the critical Re for the onset of instabilities for cylinders of aspect ratio χ . Re_{c1} and Re_{c2} are the steady and Hopf bifurcation of flow past a fixed body, whereas Re_c gives the critical Re for the onset of path instability from the experiments of Fernandes et al. [19]. Empirical fits are also provided in panel (b). The figure is adapted from Ern et al. [20].

h , the corresponding dimensional moment of inertia is:

$$I_{dim} = \frac{m}{16} \left(D^2 + \frac{4}{3} h^2 \right). \quad (2.13)$$

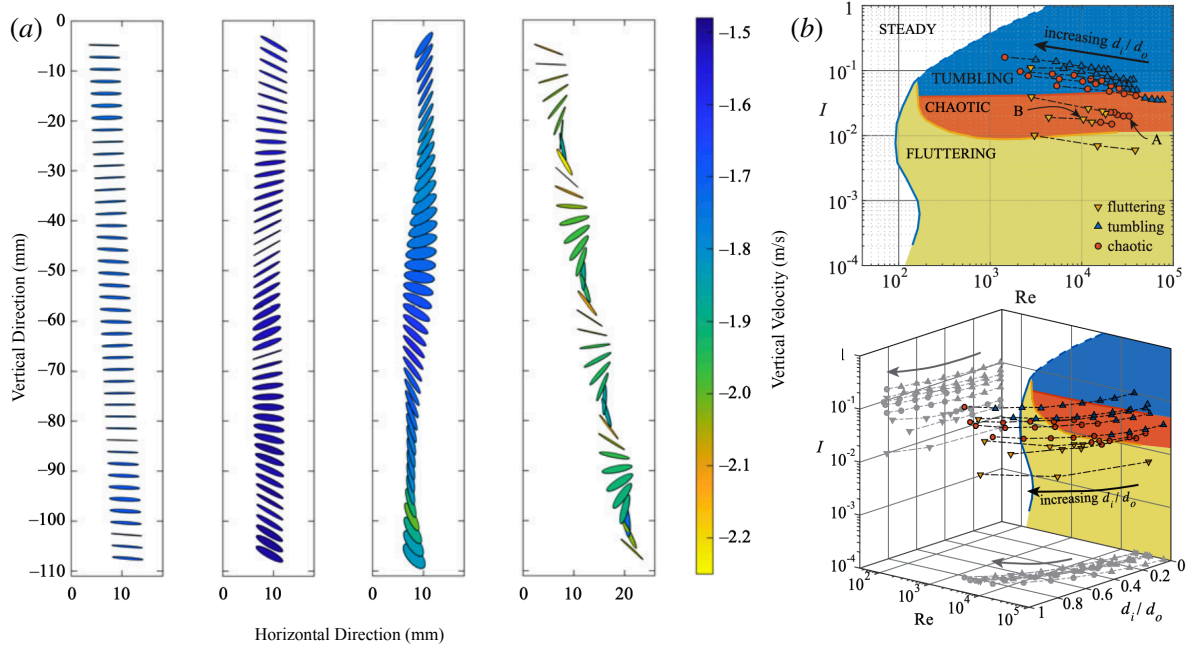


Figure 2.4: Panel (a), adapted from Tinklenberg et al. [21], presents sample trajectories for thin discs falling in air from the experiments of Tinklenberg et al. [21]. The observed regimes correspond to a straight vertical path, a small amplitude fluttering motion, a large amplitude fluttering motion, and a tumbling regime. Panel (b), adapted from Vincent et al. [22], presents the regime map for falling discs from Field et al. [23], describing the different regimes based on (Re, I) parameter space, but including the role of a central perforation on the dynamics (effect of d_i/d_o).

Non-dimensionalising I_{dim} gives:

$$I = \frac{I_{dim}}{\rho_f D^5}, \quad (2.14)$$

$$I = \frac{\rho_p}{\rho_f} \frac{\pi h}{64 D^3} \left(D^2 + \frac{4}{3} h^2 \right). \quad (2.15)$$

For rising and settling particles at moderate Reynolds numbers, Ern et al. [20] provides a comprehensive synthesis of experimental, numerical and theoretical developments on the onset of non-rectilinear trajectories. According to potential-flow arguments [18, 24], pressure drag dominates for blunt bodies, and this favours orientations that maximise the projected area normal to the direction of motion (a broadside-on orientation). However, the onset of path instability is generally attributed either to the coupling between hydrodynamic forces and torques and perturbations in the body's degrees of freedom, or to the development of a wake instability above a critical Re .

Ern et al. [20] emphasises the role of the governing parameter space, commonly ex-

pressed in terms of $(\bar{\rho}, Re, \chi)$ for rigid axisymmetric bodies, and summarises critical conditions for the onset of wake and path instabilities, including the experimental results of Fernandes et al. [19] for freely rising flat cylinders. This is illustrated in panels (a) and (b) of Fig. 2.3: panel (a) shows the parameter space, and panel (b) presents the critical Reynolds number (denoted Re_c) for the onset of path instability for cylinders with varying aspect ratios. The critical Reynolds number depends on the body geometry, since the wake structure and the associated hydrodynamic forces and torques are strongly affected by the particle shape. Beyond the onset of instability, the resulting motion is often oscillatory, characterised by a lateral displacement and a periodic vortex-shedding wake. A convenient non-dimensional measure of this oscillatory dynamics is the Strouhal number (St), defined as

$$St = \frac{fL}{U}, \quad (2.16)$$

where f is the dominant oscillation (or shedding) frequency, L is the characteristic length scale, and U is the characteristic velocity. From panel (b), it can be seen that the critical Re for the onset of path instability is strongly dependent on the aspect ratio for thick cylinders; however, this dependence plateaus once the disc is sufficiently thin. The simulations of Auguste et al. [25] found a similar dependence for the transition from a straight vertical (SV/rectilinear/steady are all different names for the same regime) regime to a zig-zag (fluttering) regime, and reported that sufficiently thin discs exhibit persistent three-dimensional regimes related to the fluttering and tumbling regimes.

In panel (a) of Fig. 2.4, four sample trajectories of a thin disc falling in air are presented from the experiments of Tinklenberg et al. [21]. The falling discs show three main regimes, the first being the SV regime, the second the fluttering regime, and the last the tumbling regime. It should be noted that the fluttering regime may correspond to either low-amplitude fluttering or large-amplitude fluttering; both are presented in the figure. In panel (b), a regime map based on (Re, I) is presented for falling discs from the work of Field et al. [23]. An additional regime is observed here, which was not reported in the experiments of Tinklenberg et al. [21], namely the chaotic regime. Furthermore, the disc dynamics is seen to transition from a fluttering regime to a tumbling regime when increasing I (at fixed Re). Therefore, decreasing I while keeping Re constant (at sufficiently large Re) is typically observed to stabilise the disc's motion.

Another contribution to stabilisation was reported in the experiments of Vincent et al. [22] at high Re , where the introduction of a central perforation altered the observed settling regime. When a central perforation is introduced, the perforation diameter plays a key role in the stabilisation process. Vincent et al. [22] found that most regime transitions

occur for $d_i/d_o \simeq 0.3 \pm 0.1$, where d_i/d_o denotes the ratio of the inner and outer diameters. However, this transition was not observed in all cases: for sufficiently large I , some cases required a much larger ratio (closer to 0.8) to induce a regime transition. The regime transition was attributed to the formation of a secondary vortex ring near the inner edge of the disc, which acts against the primary vortex ring typically observed for bluff bodies, thereby decreasing the effective circulation.

In summary, the dynamics of freely rising and settling bodies in homogeneous fluids are governed by a balance between buoyancy, inertia, and viscosity, and are strongly modulated by particle geometry. The aspect ratio χ plays a central role in setting the critical Re for the onset of path instability, with a pronounced dependence for thick cylinders that plateaus for sufficiently thin discs. Beyond χ , additional parameters that modify the observed dynamics, such as geometric modifications, including central perforations, can shift regime boundaries.

2.3 Boussinesq approximation

In the ocean, continuous stratification arises from variations in ambient temperature, salinity (concentration), and pressure, which lead to significant changes in fluid density with depth. In this section, we derive the governing equations for a stably stratified fluid in the absence of Coriolis forces.

The Boussinesq approximation assumes that variations in the ambient fluid density are negligible everywhere except in the gravitational body force term. In this approximation, other fluid properties, such as the dynamic fluid viscosity and the diffusivity of the stratifying agent, are treated as constants. The continuity equation ($\rho^{-1}(D\rho/Dt) + \nabla \cdot \mathbf{u} = 0$, where D/Dt is the material derivative defined by $D/Dt = \partial/\partial t + \mathbf{u} \cdot \nabla$), is replaced with the incompressible form found in Eq. 2.1. This does not mean that the density is constant along the motion. Rather, it assumes that density variations are small enough that their effect on the continuity equation can be neglected, while they may still be retained in the gravitational body force term. An example where this assumption breaks down is in high Mach number flows, where compressibility effects are significant and the density varies strongly with pressure.

If we assume that compressibility effects are negligible, and density variations arise due to temperature (for example) effects alone, the coefficient of thermal expansion (β)

can be defined as:

$$\beta = -\frac{1}{\rho} \left(\frac{\partial \rho}{\partial T} \right)_p, \quad (2.17)$$

where the subscript p means that the variation is taken under constant pressure. Using the linearised equation of state (valid for $|\beta(T - T_0)| \ll 1$), the fluid density field is written as:

$$\rho_f(\mathbf{x}, t) = \rho_0 \left[1 - \beta(T(\mathbf{x}, t) - T_0) \right], \quad (2.18)$$

where $\rho_0 = \rho(T_0)$ is the reference density at the reference temperature T_0 . Typical values of the thermal expansion coefficient β can be found in standard references [26]. For a perfect gas, $\beta = 1/T$, so at $T \approx 300$ K one has $\beta \sim 3 \times 10^{-3} \text{ K}^{-1}$, whereas for liquids β is typically $\sim 5 \times 10^{-4} \text{ K}^{-1}$.

Let ρ , and p^a be decomposed into a hydrostatic reference state plus perturbations (denoted by primes):

$$\rho = \rho_0 + \rho', \quad p^a = p_0^a + p'. \quad (2.19)$$

Assume the reference density ρ_0 is constant and the reference pressure $p_0^a(z)$ satisfies hydrostatic balance:

$$\nabla p_0^a = \rho_0 \mathbf{g}. \quad (2.20)$$

If we subtract the reference state from Eq. 2.2 and divide by ρ_0 :

$$\left(1 + \frac{\rho'}{\rho_0}\right) \frac{D\mathbf{u}}{Dt} = -\frac{1}{\rho_0} \nabla p' + \frac{\rho'}{\rho_0} \mathbf{g} + \nu \nabla^2 \mathbf{u}, \quad (2.21)$$

where $\nu = \mu/\rho_0$ is the kinematic viscosity. It can be seen from Eq. 2.21 that ρ'/ρ_0 appears in both the inertial and buoyancy terms. If $|\rho'|/\rho_0 \ll 1$, its contribution to the inertial term is negligible and may be omitted. However, it must be retained in the buoyancy term, since even small density variations generate a non-negligible gravitational force, yielding:

$$\frac{D\mathbf{u}}{Dt} = -\frac{1}{\rho_0} \nabla p' + \frac{\rho'}{\rho_0} \mathbf{g} + \nu \nabla^2 \mathbf{u}. \quad (2.22)$$

The continuity and momentum equations are then coupled with a transport equation for the stratifying agent, which reads:

$$\frac{DT}{Dt} = \kappa \nabla^2 T, \quad (2.23)$$

where κ is the thermal diffusivity.

These equations are valid for a fluid with small density variations ($|\rho'|/\rho_0 \ll 1$), provided that the Mach number is small and the characteristic vertical length scale is

not too large. Lastly, for an impermeable particle suspended in a density-stratified fluid, a no flux (insulating) boundary condition for the temperature at the particle surface is typically imposed:

$$\mathbf{n} \cdot \nabla T = 0, \quad (2.24)$$

which corresponds to an adiabatic particle. This boundary condition is an idealised assumption for a thermally stratified fluid, such that the particle conductivity is negligible compared with that of the ambient fluid, an approximation that remains appropriate for microplastics (which have negligible thermal diffusivity). If the stratifying agent is, for instance, salinity rather than temperature, then this boundary condition is appropriate.

2.4 Particle dynamics in density-stratified fluids

In a density-stratified fluid, an inviscid fluid element displaced from its neutrally buoyant (equilibrium) position undergoes simple harmonic oscillations with buoyancy frequency N . This buoyancy frequency, typically called the Brunt-Väisälä frequency, is defined as:

$$N^2 = -\frac{g}{\rho_0} \frac{d\rho}{dz}, \quad (2.25)$$

where $\frac{d\rho}{dz} < 0$ characterises the stable ambient stratification. A displaced fluid element moves along an isopycnal (a surface of constant density), while the resulting oscillations are progressively damped in a viscous fluid. In the context of freely moving particles in density-stratified fluids, isopycnal displacement arises from the entrainment of ambient fluid induced by the particle's motion. Due to the no flux boundary condition, the distorted isopycnals finish orthogonal to the particle surface. The buoyancy force tends to restore displaced fluid elements toward their equilibrium position, generating internal waves, commonly referred to as lee waves when they form in the wake of a suspended obstacle.

It is therefore useful to introduce additional dimensionless numbers that govern the dynamics of particles in a stratified fluid. The strength of the stratification may be characterised by the Froude number ($Fr = U/(NL)$). The diffusivity of the stratifying agent is characterised by the Prandtl number (Pr) or the Schmidt number (Sc), which compares the momentum diffusivity to the thermal diffusivity and the mass diffusivity (ν/κ), respectively. In this work, Pr and Sc are used interchangeably to denote the ratio of momentum diffusivity to scalar diffusivity, with Pr corresponding to temperature stratification and Sc to solutal stratification. In addition, the Péclet number may be

defined as follows:

$$Pe = RePr = \frac{UL}{\kappa}, \quad (2.26)$$

which is the ratio between advective and diffusive transport. Typical values are $Pr = 0.7$ for a thermally stratified atmosphere, $Pr = 7$ for thermally stratified water, and $Sc = 700$ for salt stratified water.

The focus of this thesis is on the dynamics of particles that settle or rise in an ambient stratification in the moderate Re regime. Previous works have addressed the low Re regime ($Re \ll 1$), and a review of these studies can be found in More and Ardekani [11]. If we consider a particle settling or rising in the ocean, the vertical length scales over which the ambient density varies can greatly exceed those accessible in laboratory experiments and numerical simulations. It is therefore common to model the background stratification using idealised profiles, most often either a linear stratification or a sharp, two-layer stratification separated by a transition layer. A linear model is particularly useful when considering a stratification vertical scale much larger than the length scale associated with the particle.

2.4.1 Flow field and transient behaviour

As a particle settles (rises), it entrains a parcel of lighter (heavier) ambient fluid in its wake and near-surface boundary layer, altering the effective inertia and buoyancy of the particle, thereby modifying the observed dynamics. This entrainment establishes a scalar (diffusive) boundary layer adjacent to the particle, in addition to the momentum boundary layer, with a thickness set by the diffusivity of the stratifying agent. Previous studies have provided estimates of the thickness of these boundary layers by performing a first-order balance depending on the regime [27]. A summary of these estimates is provided in table 2.1.

At finite Re , the entrained fluid is advected along the particle surface within the boundary layer to the rear stagnation point, where it forms a jet that transports the fluid back toward its neutrally buoyant level. The jet is typically identified as the region immediately behind the particle characterised by large vertical velocities directed opposite to the particle's motion. The strength of the jet is directly related to the non-dimensional parameters (Re , Fr , Pr), as seen from the simulations of Zhang et al. [14] presented in panel (a) of Fig. 2.5. As Fr decreases, entrained fluid parcels undergo a larger increase in potential energy, so the exchange between potential and kinetic energy becomes stronger (governed by the buoyancy flux). As a result, the jet intensifies as Fr decreases. Further-

Table 2.1: Dimensionless momentum (δ_m) and diffusive (δ_ρ) boundary layer thickness estimates from the literature [11, 27].

Regime	δ_m	δ_ρ
$Re \ll 1$	Re^{-1}	$\begin{cases} Pe^{-1}, & Pe \ll 1, \\ Pe^{-1/3}, & Pe \gg 1, \end{cases}$
$10^{-2} \leq Re \leq 10^2$ $(10 \leq Pe \leq 10^6)$	$\begin{cases} \mathcal{O}(1), & Fr \geq 10, \\ Fr^{1/2} Re^{-1/2}, & Fr < 10, \end{cases}$	$\begin{cases} Pe^{-1/3}, \\ Fr^{1/6} Re^{-1/6} Pe^{-1/3}, \\ Re^{-1/2} Pr^{-1/3}, & Pr \gg 1, \\ Re^{-1/2} Pr^{-1/2}, & Pr \ll 1 \end{cases}$
$Re \gg 1$	$Re^{-1/2}$	

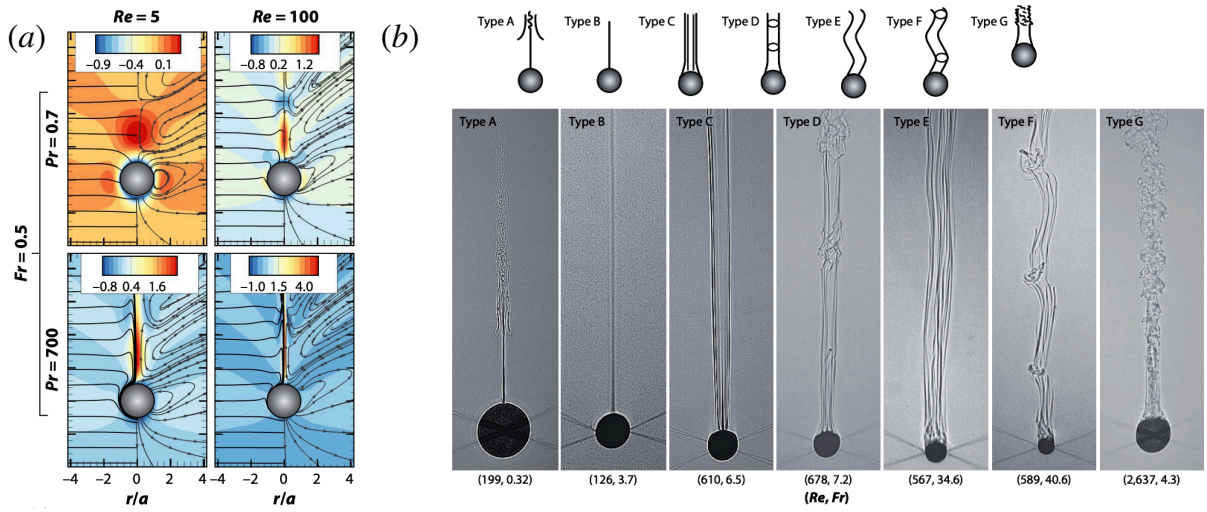


Figure 2.5: Panel (a) shows the simulations of Zhang et al. [14] for a settling sphere in a linearly stratified fluid and changing the underlying dimensionless numbers. Panel (b) shows the different wake patterns found for a settling sphere in a linearly stratified fluid from the experiments of Hanazaki et al. [28]. The figure has been adapted from More and Ardekani [11].

more, as Pr decreases, scalar diffusion acts more readily, producing a wider vertical jet with lower velocity magnitudes. Increasing Re strengthens the wake, typically increasing the amount of entrained fluid and yielding a more pronounced, coherent rear jet with larger velocity magnitudes. In panel (b), the experiments of Hanazaki et al. [28] show the different wakes observed for a settling spherical particle when varying Re and Fr for $Sc = 700$. The observed wake morphologies are:

- *Type A*: slender jet exhibiting a pronounced bell-like envelope produced by the internal waves. The length of the jet (from the rear stagnation point to the lowest part of the bell) increases with Fr .

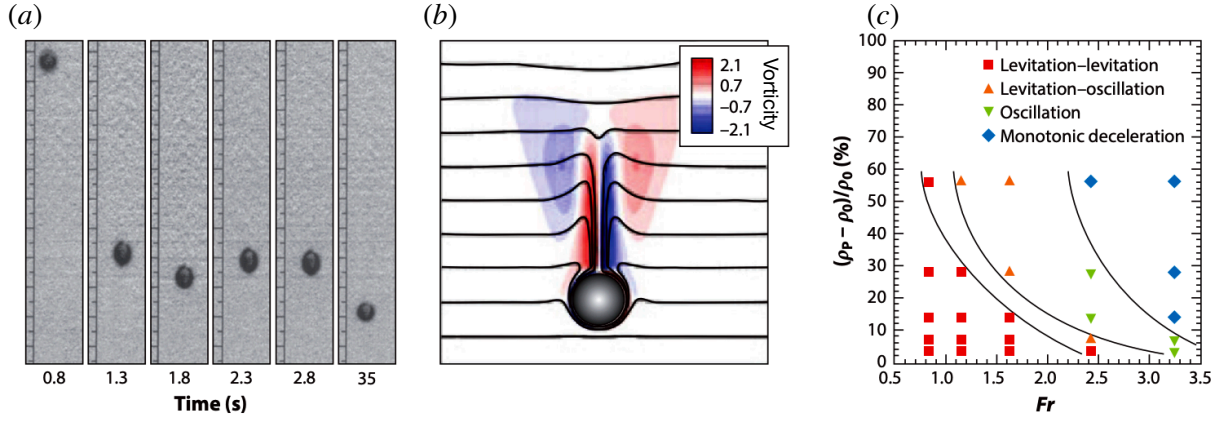


Figure 2.6: Panel (a) shows the levitation behaviour found for a sphere settling through a sharp density transition layer from the experiments of Abaid et al. [29]. In panel (b), the flow field of a sphere settling in a linearly stratified fluid is presented highlighting the vorticity profile and the distorted isopycnals from the simulations of Doostmohammadi et al. [30]. In panel (c), a regime map for the settling behaviour from the simulations of Doostmohammadi et al. [30] is presented when ($Re = 353$, $Sc = 700$) and varying Fr . The figure is adapted from More and Ardekani [11].

- *Type B*: thin, elongated jet that remains essentially rectilinear when slightly increasing Fr .
- *Type C*: wide, steady jet persisting over a long distance at moderate Re and Fr . The width of the jet increases with increasing Fr , and is controlled by stratification, not by the boundary layer separation.
- *Type D*: broad jet that is time-dependent and develops regularly spaced knots; the characteristic period depends on Fr , indicating control by the stratification but not a consequence of internal waves.
- *Type E*: weakly meandering broad jet that does not form distinct knots.
- *Type F*: knotted jet related to the vortex shedding behaviour found in homogeneous fluids (large Re and Fr).
- *Type G*: fully turbulent jet arising for $Re > 10^3$.

Recent three-dimensional DNS by Mo et al. [31] investigated the onset of three-dimensionality in the Type A jet as Fr is decreased. They showed that the transition is driven by the coupling between the vorticity profile and the stratification-modified wake. The vorticity equation may be derived by taking the curl of the momentum equation for

a density-stratified fluid:

$$\frac{D\boldsymbol{\omega}}{Dt} = (\boldsymbol{\omega} \cdot \nabla)\mathbf{u} + \frac{\mu}{\rho_0} \nabla^2 \boldsymbol{\omega} + \nabla p \times \nabla \left(\frac{1}{\rho} \right), \quad (2.27)$$

where $\boldsymbol{\omega}$ is the vorticity. The last term on the right-hand side of Eq. 2.27 is the baroclinic torque term, responsible for vorticity generation when pycnoclines are displaced in a density-stratified fluid. This form of the baroclinic source term may be rewritten under the Boussinesq approximation as $-(g/\rho_0)(\nabla\rho \times \mathbf{e}_z)$, where $\mathbf{e}_z$ is the vertical unit vector. This means that any radial (horizontal) density gradient created by distorted isopycnals generates azimuthal vorticity. Below a critical Froude number, the baroclinic torque term drives the collapse of the standing toroidal eddy observed in a homogeneous fluid, as shown by Torres et al. [32]. Panel (b) of Fig. 2.6 shows a representative simulation of a settling sphere in a density-stratified fluid from Doostmohammadi et al. [30], with the background vorticity field. In the wake of the sphere, secondary and tertiary toroidal vortices form with opposite sign to the primary vortex ring near the sphere, induced by the no-slip condition at the particle surface. These additional wake vortices arise as the distorted isopycnals return back toward their equilibrium position, as indicated by the density contours, and this adjustment is accompanied by the formation of internal waves.

For a settling particle in the weakly stratified limit (large Fr), the settling velocity depends only weakly on the ambient stratification. For particles whose density is close to that of the ambient fluid, such as plastics in the ocean, a wide range of transient dynamical behaviours can arise. In contrast to particles in a homogeneous fluid, particles in a linearly stratified fluid generally do not attain a constant terminal vertical velocity because the buoyancy force varies with the vertical position of the particle. Instead, the particle decelerates and comes to rest once it reaches its equilibrium depth. Typically, a spherical particle that settles ($\rho_p > \rho_0$) in a linearly stratified quiescent fluid accelerates from rest until it reaches a velocity magnitude peak. After that, the particle starts to decelerate as the impact of buoyancy and stratification-induced drag increases, discussed in Section 2.4.4. Furthermore, when increasing Fr , thereby decreasing the stratification strength, the peak velocity magnitude attained by the particle increases. During particle deceleration, several different regimes were found by Doostmohammadi et al. [30], presented in panel (c) of Fig. 2.6. When Fr is large, a monotonic deceleration is typically found. On the other hand, increasing the stratification strength, oscillation of the particle's vertical velocity is observed. The amplitude of the oscillation increases with decreasing Fr , and the oscillation frequency scales with N . This suggests that the oscillatory behaviour is tied to the internal waves generated by the particle's motion, which are tightly related to the baroclinic source term discussed earlier.

Furthermore, when considering the role of Pr , increasing the diffusivity of the stratifying agent (decreasing Pr) reduces the intensity of the baroclinically generated vorticity. Although this can strongly influence the surrounding flow field, its impact on the vertical velocity of the particles is relatively small in the monotonic deceleration regime. However, because the oscillatory regime is linked to the coupling between the forces on the particle and the internal waves radiated in the wake, decreasing Pr typically leads to weaker oscillations in the vertical velocity of the particle [30]. Upon further decreasing Fr , a levitation regime may also be encountered. This regime is characterised by a transient reversal of the particle motion, even though the particle remains denser than the ambient fluid at that vertical position. Such reversals were first reported in the experiments of Abaid et al. [29] for a sharply stratified fluid, shown in panel (a) of Fig. 2.6.

More recently, Camassa et al. [33] and Wang et al. [34] have examined the bouncing dynamics of spheres in sharply stratified fluids using potential energy and force balance arguments, respectively. In panel (c), an overview of the different regimes found by the simulations of Doostmohammadi et al. [30] in a linearly stratified fluid is presented when $Re = 353$ and $Sc = 700$. It should be noted that fully resolving the diffusive boundary layer in this regime using three-dimensional DNS is a computationally intensive task, as the levitation regime is mainly found when (Re, Sc) is large.

2.4.2 Particle shape and porosity

When considering the role of particle geometry, previous work for settling impervious discs [37, 38] and spheroids [35, 39] at moderate Re has shown their tendency to reorient from the broadside-on orientation to an edgewise orientation under strong stratification. Reorientation was found to be related to the dominance of the buoyancy induced torque over the hydrodynamic torque [35]. At higher Reynolds numbers, Lam et al. [40] have shown that the buoyancy torque may also dampen the orientation dynamics of fluttering discs. Moreover, stratification tends to prohibit the lateral motion observed for discs and spheroids found in homogeneous fluids beyond a critical Reynolds number [19, 41]. In a linearly stratified fluid, More et al. [35] found that the settling dynamics can be separated into three distinct phases, illustrated in panel (a) of Fig. 2.7. First, there is a broadside settling regime in which the particle follows a rectilinear path. As the spheroid settles, it encounters a denser fluid until the magnitude of the destabilising buoyancy torque dominates over the stabilising inertial torque, leading to particle reorientation. An oblate spheroid was found to attain a fully edgewise orientation in the last phase, namely, phase (iii), whereas a prolate spheroid attains an intermediate angle between broadside-on and

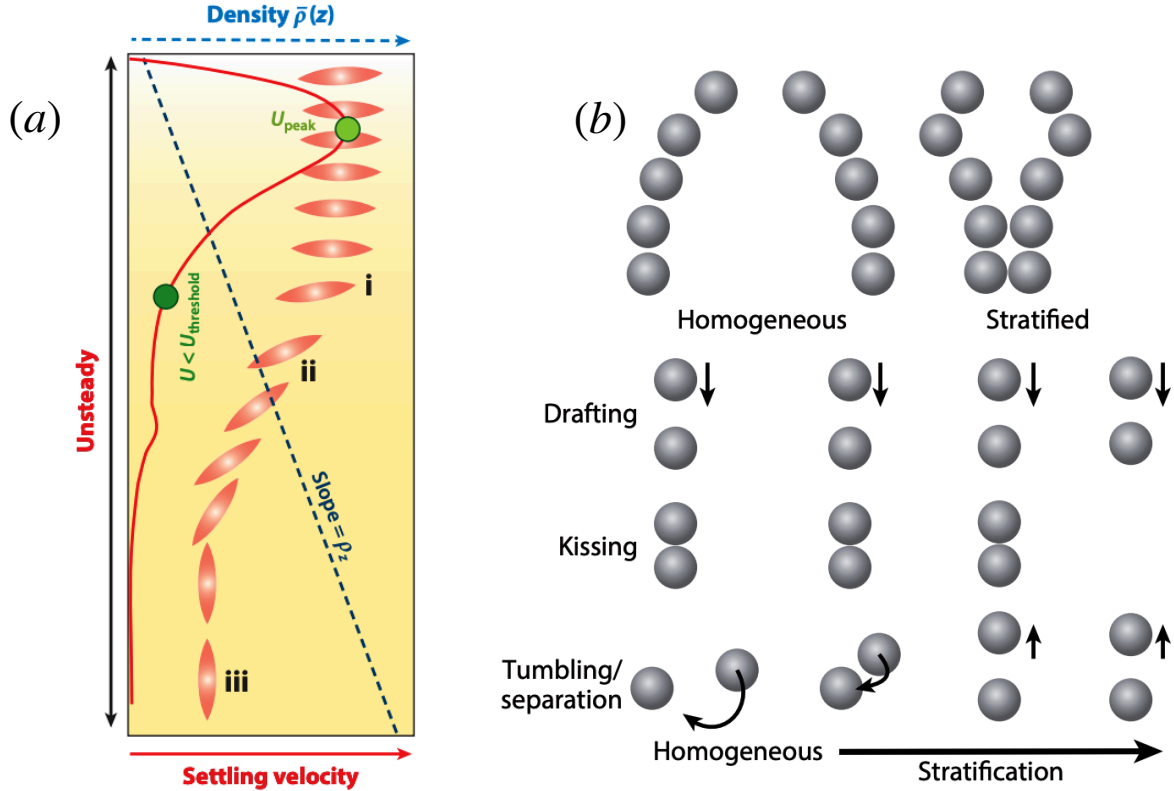


Figure 2.7: An illustration of the reorientation behaviour of a settling spheroid in a linearly stratified fluid is presented in panel (a), as seen from the work of More et al. [35]. In panel (b), and illustration of the interaction between a spherical particle pair in a homogeneous and density-stratified fluid is presented in both the side-by-side and in-line configurations. The figure is adapted from More and Ardekani [11] and Ardekani et al. [36].

edgewise.

Mercier et al. [37] reported similar behaviour for settling impervious discs in a linearly stratified fluid at moderate Re , and Mrokowska [38] observed the existence of five distinct phases when a disc crosses a sharp density transition. As the disc approaches the sharp density transition, it reorients to an edgewise configuration; once it enters the second homogeneous layer, it returns to a broadside orientation. In general, as the particles reorient in a stratified fluid, they glide horizontally as the reorientation induces a lift force. The role of particle shape anisotropy on the rising and settling dynamics in a stratified fluid is far from being fully understood, as most studies have considered idealised shapes and isolated particles to investigate the dynamics.

Unlike impermeable particles, porous bodies such as marine snow satisfy the usual no-slip and no-penetration conditions for the velocity at their surface, yet the stratifying agent can still diffuse through the pore space. This diffusive exchange allows the particle's

effective density to change as it settles through a stratified layer, which can strongly modify its settling path and its residence near density interfaces.

For highly porous bodies, the dynamics enters a diffusion-limited regime, in which diffusion through the pore space controls how rapidly the particle adjusts to the surrounding stratification. The effective density of the particle is determined by the combined contributions of the solid matrix and the pore fluid, and can evolve as the pore fluid equilibrates with the local ambient density. Therefore, accumulation in a density-transition layer is possible when the density jump across the interface is large enough, relative to the excess density of the particle, that only a small change in the pore-fluid density is needed to bring the particle close to neutral buoyancy.

A key consequence of this diffusion-limited behaviour is a pronounced particle size dependence. Because the equilibration of the interstitial fluid is controlled by diffusion, larger particles adjust more slowly to changes in the ambient density field, and therefore can remain out of equilibrium for longer as they approach and traverse the interface. This slower adjustment can delay the attainment of neutral (or near-neutral) buoyancy and prolong the interaction with the pycnocline, effectively increasing the residence time in the vicinity of the density transition. Consistently, simulations in the same diffusion-limited regime show that the residence time of porous spheres at pycnoclines increases logarithmically with the Péclet number [42].

2.4.3 Particle-particle interactions

Recent works [16, 46, 47] have shown that two spherical particles, initially separated by a distance of $\mathcal{O}(D_p)$, settling side-by-side in a density-stratified fluid experience mutual attraction due to the formation of a reverse jet in the gap region between them. In contrast, when particles are initially aligned vertically, the trailing particle experiences an initial acceleration towards the leading particle, a phenomenon known as *drafting*, followed by a separation under strong stratification. An illustration highlighting these two behaviours is presented in panel (b) of Fig. 2.7. This behavior differs markedly from the case of a homogeneous fluid, where an initially horizontal pair experiences a hydrodynamic repulsion caused by the particles' disturbance velocity field outside their wakes. In the vertical arrangement, drafting can bring the particles into contact, triggering the so-called '*kissing*' stage: as the trailing particle catches up, the parallel alignment is disrupted by their collision, leading to perturbations in their positions. If these disturbances are sufficiently large, the particles may tumble, exchanging leading and trailing roles before

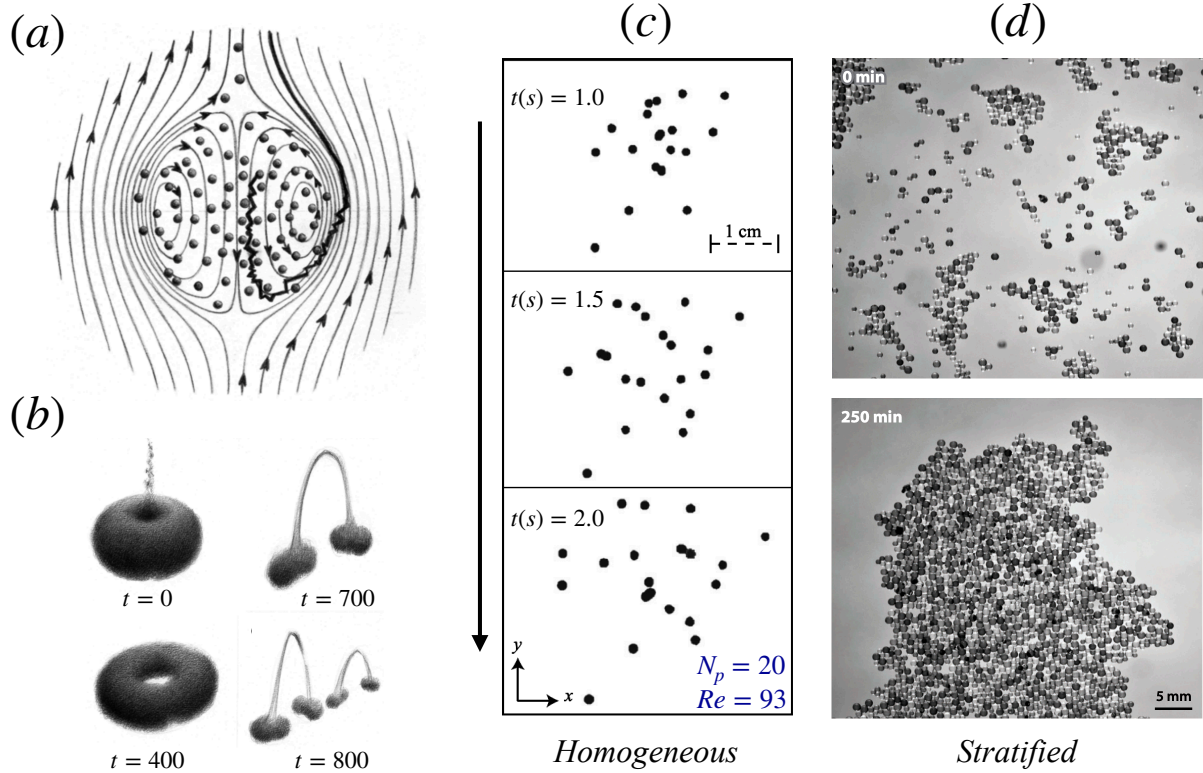


Figure 2.8: Panel (a) shows a Hadamard–Rybczynski type toroidal circulation throughout the particle cloud volume, with the moving reference frame streamlines. In panel (b), the disintegration of a particle cloud into a torus, and further into daughter droplets in a cascade is presented. Panels (a) and (b) are adapted from Guazzelli and Morris [17] and Guazzelli [43], respectively. A top view spatio-temporal evolution of the interaction between spherical particles initialised as a sparse cluster is presented in panel (c) from the experiments of Daniel et al. [44] with $N_p = 20$ and $Re = 93$, where N_p is the number of particles. In panel (d), the spatio-temporal evolution of a spherical particle cluster of neutrally buoyant particles in a sharply stratified fluid from the experiments of Camassa et al. [45], highlighting their self assembly.

settling resumes [48].

In the case of a dilute suspension of spherical particles, Doostmohammadi and Ardekani [49] and Deepwell and Sutherland [50] have shown that the magnitude of the sedimentation velocity decreases compared to the case of homogeneous fluid, and stratification tends to reduce the size of the groups due to induced upward flows in the wake of settling particles. Moreover, the particles become more vertically aligned at larger Sc due to the increased strength of the jet behind the advancing cluster. Furthermore, for a group of spherical particles initially suspended at a neutrally buoyant level in a sharply stratified fluid, the particles can undergo self-assembly, as shown in panel (d) of Fig. 2.8. As reported by Camassa et al. [45], this behaviour is diffusion-induced: solute diffusion

constrained by the no-flux condition at the particle surfaces drives toroidal circulations that produce an effective horizontal attraction, promoting clustering and the formation of coherent structures. Although a few studies have examined the interaction of spherical particle pairs and the sedimentation of dilute suspensions of spheres in density-stratified ambients, a gap remains in our understanding of how particles of different geometries interact in such environments and how their behaviour compares directly with that of spheres in a homogeneous fluid.

In homogeneous fluids, particle suspensions and particle clouds have been studied in both viscous and inertial regimes; see, for example, the recent review of Fardin et al. [51]. In the viscous regime (Stokes), Nitsche and Batchelor [52] showed that a sedimenting cloud of spherical particles, which can be modelled in the far field as a Stokeslet, largely preserves its initial shape while the particles steadily escape from the rear, eventually leading to cloud disintegration. The internal motion is characterised by a Hadamard–Rybczynski type toroidal circulation throughout the cloud volume, which advects particles towards the trailing end, as seen in panel (a) of Fig. 2.8. Superposed on this toroidal motion, hydrodynamic interactions between particles generate random displacements. These fluctuations can drive particles across the cloud boundary into regions with negligible particle concentration. Outside the cloud, streamlines sweep around the cloud surface and are no longer closed, instead extending to infinity. Particles carried around to the rear then lag behind the faster-moving cloud and do not re-enter it, forming a trailing tail. Analogies with a falling drop with negligible surface tension have also been discussed, for example, by Guazzelli [43], where the drop radius is taken to be the cluster radius R_c .

The stability of the cloud depends on the particle number N_p : as N_p increases, the initially compact cluster becomes unstable, deforms into a toroidal shape, and then undergoes a repeating breakup in which the torus ‘pinches off’ into two daughter drops in a repeating cascade (see panel (b) of Fig. 2.8). The transition to the macro-scale inertial regime occurs once the cloud Reynolds number increases to $Re_{cl} = O(1)$. A further transition to the micro-scale inertial regime occurs when inertia at the particle scale becomes important on the scale of the cloud, so that the Oseen disturbances (or wakes) generated by individual particles reach the cloud boundary and interact with it. In the Oseen regime, Subramanian and Koch [53] showed that this happens when the inertial screening length, which scales like D_p/Re , is comparable to the cloud radius R_c (with Re based on the particle diameter D_p). Under these conditions, an initially spherical particle cluster with a number of particles N_p smaller than $\mathcal{O}(R_c^0 U/\nu)$, where R_c^0 is the initial cluster radius, is expected to expand while retaining a spherical shape due to limited wake-mediated interactions. When N_p is much larger than $\mathcal{O}(R_c^0 U/\nu)$, the probability of wake-mediated

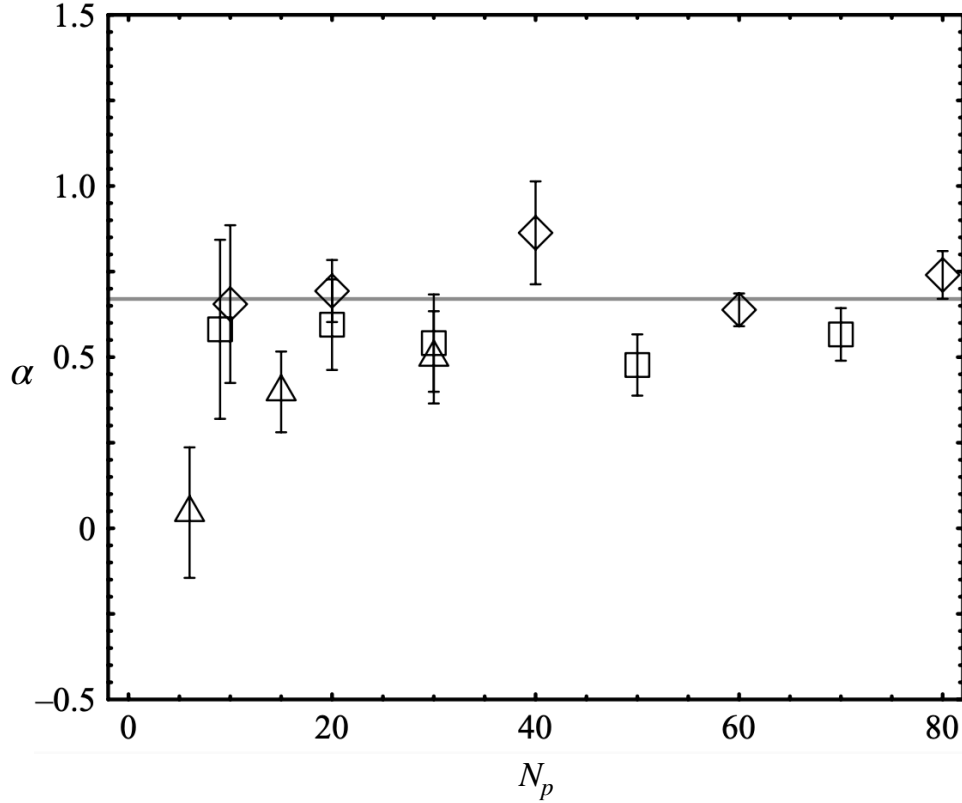


Figure 2.9: Growth exponents for the evolution of spherical particle cluster where $\langle r_t^2 \rangle = t^\alpha$ when varying N_p and Re from the experiments of Daniel et al. [44]. The solid line corresponds to $\alpha = 2/3$, and the marker shapes are: $Re = 93$ ($\diamond$), $Re = 216$ ($\square$), $Re = 425$ ($\triangle$).

interactions increases, leading to the evolution from a spherical cluster to a quasi-planar cluster. The cluster variance for all times for the former case, and long times for the latter case (after an initial quadratic growth), is expected to grow as $\langle r_t^2 \rangle \sim t^{2/3}$ based on hydrodynamic repulsion between particles, where $\langle r_t^2 \rangle$ is the (transverse) cluster variance. This scaling was demonstrated by Subramanian and Koch [53] using self-similar solutions. Although this scaling for the time evolution of the cluster variance was initially found in the low Re limit, it was surprising to find from the experiments of Daniel et al. [44] at high Re that this scaling remains valid (see panel (c) of Fig. 2.8 which presents a top view of the time history for the particle configuration). The low- Re theory was further extended to higher Re by incorporating an empirical correlation for the drag on a falling sphere, demonstrating the robustness of this scaling. In Fig. 2.9, the experimental results of Daniel et al. [44] for the growth exponent α are shown as the initial number of particles in the cluster, N_p , is varied. Although the theory is derived for a continuum description of a settling cluster in terms of a number-density field, good agreement is obtained even for moderate N_p .

2.4.4 Drag Enhancement

For a particle that settles or rises in a density-stratified fluid, previous studies have shown that its drag is enhanced by stratification compared to that in the homogeneous fluid case. This enhancement may be expressed in terms of the drag coefficient as $\Delta C_D = C_D^S - C_D^H$, where C_D^S denotes the (total) drag coefficient in the stratified fluid and C_D^H is the corresponding value in an otherwise homogeneous fluid. The additional drag increases with increasing $1/Fr$, and has been reported to increase by several orders of magnitude in sufficiently strong stratification [14, 35, 37].

The drag enhancement can be decomposed into three contributions: (i) an additional Archimedean component associated with entrainment, (ii) an inertial contribution arising from the momentum flux associated with density disturbances, and (iii) an additional shear force on the particle surface associated with baroclinically generated vorticity. Among these, the inertial contribution is typically the smallest [14], while the dominant contributions are linked to the misalignment between the pressure and density gradients, through entrainment and vorticity generation. The entrainment contribution to the added drag was estimated using semi-empirical modelling of Yick et al. [54]; however, Zhang et al. [14] showed that the vorticity-related contribution cannot, in general, be neglected. Regime-dependent scalings for the three contributions were reported by Zhang et al. [14] and summarised in the review of More and Ardekani [11].

For a spherical particle, and assuming Pr is fixed, the total drag coefficient may be written as [37, 55, 56]:

$$C_D^S = C_D^H(1 + aRe^p Fr^q), \quad (2.28)$$

where a , p , and q are constants. At low Re , Zvirin and Chadwick [57] found a power-law dependence with $p = 1/3$ and $q = -2/3$, while Candelier et al. [58] reported that $p = 1/4$ and $q = -1/2$ are also possible. Several other studies have found that $p = 1/2$, $q = -1$, and $a \simeq 1.9$ provide a good description of spherical particles [54, 55], while Bayareh et al. [59] reported $q = -2.8$ and $a \approx 21$ of a rising drop in a linearly stratified fluid.

It is worth noting that, under the form in (2.28), the viscous Richardson number, defined as $Ri = Re/Fr^2$, becomes a particularly relevant parameter for quantifying drag enhancement. For impervious discs, Mercier et al. [37] introduced an additional contribution of χ in (2.28), such that $C_D^S/C_D^H - 1 \sim (1 + 2/\chi)Re^{1/2}Fr^{-1.2}$, indicating that discs experience stratification-induced drag enhancement more severely than spherical particles.

In this thesis, the stratification induced drag enhancement is reported relative to

the homogeneous-fluid value as $C_D^S - C_D^H$, where C_D^H is estimated using an appropriate empirical correlation.

2.5 Particles, drops and bubbles

In immiscible fluid systems, the two phases are separated by an interface: a thin transition region across which material properties (such as density and viscosity) vary abruptly. At macroscopic scales this region is usually idealised as a sharp surface of negligible thickness, endowed with an interfacial tension. Microscopically, interfacial tension originates from the fact that molecules at the interface experience an asymmetric environment relative to those in the bulk, placing them in a higher-energy state. As a result, the system tends to reduce its interfacial area in order to lower its free energy. Equivalently, interfacial tension may be viewed as (i) an isotropic in-surface contractile stress (a force per unit length) that resists stretching or (ii) the free-energy cost per unit area associated with increasing the interfacial area. In continuum models, this capillary effect provides a restoring force and allows jumps in normal stress across the interface, thus shaping the deformation, stability, and dynamics of multiphase flows. Building on this description of fluid interfaces, we briefly introduce the dynamics of rising bubbles and drops. An overview of how suspended particles interact with multiphase flows is provided.

The motion of a gas bubble in an otherwise quiescent fluid has been studied for a long time and remains of considerable importance owing to its ubiquity in natural and industrial settings. When considering the problem of a rising bubble, the dynamics are governed by the interplay between buoyancy, viscous stresses, surrounding fluid inertia, and capillarity and are further influenced by the density and viscosity ratios and the cleanliness of the interface. These competing effects determine both the rise speed and the bubble morphology and give rise to distinct dynamical regimes: small bubbles typically remain nearly spherical, intermediate bubbles deform into oblate shapes, and larger bubbles enter regimes in which deformation is pronounced. The discussion here is not intended to be exhaustive; instead, it provides a brief introductory overview of the key ideas and a selection of representative studies.

A useful description is obtained by introducing non-dimensional parameters that compare the relevant physics. The Galilei number, $Ga = \rho g^{1/2} L^{3/2} / \mu$, is typically used to quantify the relative importance of buoyancy-driven inertial effects to viscous effects. Additionally, the relative importance of buoyancy and capillarity is commonly quantified by

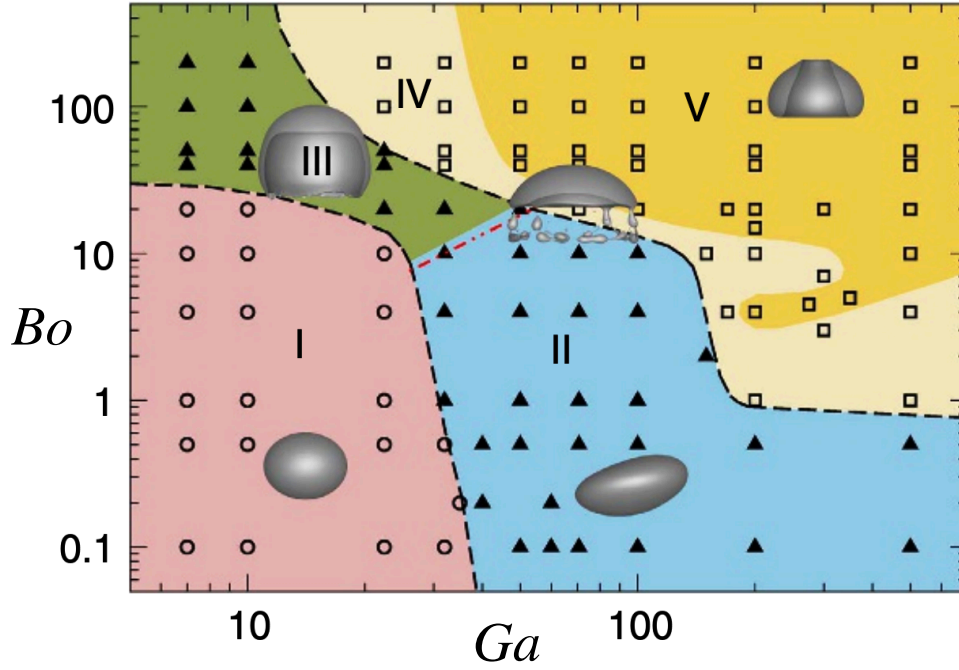


Figure 2.10: Regime map characterising the dynamics of a rising bubble in a homogeneous fluid when varying (Bo, Ga) . The regime map is adopted from Tripathi et al. [60]. The regimes are: (I) an axisymmetric bubble at small Ga and small Bo ; (II) a spiralling bubble at large Ga and small Bo ; (III) a skirted spherical-cap bubble at small Ga and large Bo ; and, at large Ga and large Bo , (IV) peripheral breakup or (V) central breakup.

the Bond (or Eötvös) number. The Bond number may be written as:

$$Bo = \frac{\Delta\rho g L^2}{\gamma}, \quad (2.29)$$

where $\Delta\rho$ is the density difference between the two phases, and γ is the surface tension. When considering rising bubbles in water, the density ratio is typically taken as $\bar{\rho} = \rho_b/\rho_f \approx 10^{-3}$, whereas the viscosity ratio $\bar{\mu} = \mu_b/\mu_f \approx 10^{-2}$. However, droplets typically exhibit a density contrast with the surrounding fluid much smaller than that of gas bubbles, and their viscosity is often comparable to, or greater than, that of the ambient phase.

The effective mobility of the bubble surface is determined by the tangential component of the interfacial stress balance. For a clean interface (in the absence of contaminants such as surfactants), the tangential stress is continuous, whereas even small amounts of surfactants can immobilise the interface through Marangoni stresses. These effects can lead to large changes in drag and rise speed and underpin much of the observed variability in bubble dynamics across different fluids and experimental conditions.

Turning to regime classification, Tripathi et al. [60] conducted three-dimensional DNS of a bubble rising in an otherwise quiescent Newtonian fluid. They agreed well with the experiments of Bhaga and Weber [61], and identified five distinct regimes in the parameter space (Ga, Bo) : (I) an axisymmetric bubble in small Ga and small Bo ; (II) a spiralling bubble in large Ga and small Bo ; (III) a skirted spherical-cap bubble in small Ga and large Bo ; and, at large Ga and large Bo , (IV) peripheral breakup or (V) central breakup. These regimes are presented in Fig. 2.10. More complex configurations have also been considered in the literature, including interactions between bubble pairs [62–64], the effects of viscosity stratification in the ambient fluid [65], and the presence of surfactants [66].

Furthermore, Bayareh et al. [59] studied the effects of a linearly stratified fluid on the rising motion of a deformable drop. The study showed that as the drop increases, the drop to fluid density contrast decreases, reducing the drop velocity, similar to the case of a rigid particle. Furthermore, stratification leads to differences in the flow structure. These effects were found to decrease the pressure difference between the centre of the drop and the surface of the drop, reducing the drop deformation frequently seen in a homogeneous fluid. The role of Marangoni stresses arising from concentration or temperature gradients in the dynamics of droplets in density-stratified fluids has also been investigated [67]. The resulting flow is governed by competition between Marangoni convection (driving motion from regions of low γ to regions of high γ), buoyancy effects, and diffusion. In this setting, Li et al. [67] reported striking unsteady behaviour, in which droplets undergo sustained oscillations through repeated bouncing. This periodic motion reflects the continual build-up and relaxation of interfacial-tension gradients as the droplet migrates through the stratification, with diffusion acting to attenuate these gradients over time. Such findings highlight that interfacial stresses can generate strongly time-dependent trajectories in stratified media and must therefore be taken into account when assessing droplet transport and residence times. When bubbles are considered in stratified fluids, less work has been done compared to droplets in such environments [11]. Bubbles tend to deform more readily in comparison, and the interaction between bubble swarms and the ambient fluid can improve mixing, potentially leading to destratification [11, 68, 69]. Further discussion of droplets and bubbles in stratified media can be found in [11, 12, 70, 71].

Bubbles rising in the ocean can also interact with sedimenting particles, which can play a role in their transport [72]. At the core of these interactions is the dynamic behaviour of bubbles. When a bubble impacts and interacts with a horizontal [73–75] or curved [76, 77] solid surface, a hydrodynamic dimple [78] might form on the surface of the bubble closest to the solid boundary. If the approach velocity of the interaction is sufficiently high, the bubble may rebound or bounce after colliding with the solid surface

[79–81]. If the approach velocity is low, a trapped liquid film in the gap region between the bubble and the solid surface will start to drain. Klaseboer et al. [82] and Chan et al. [79] have studied the film drainage and coalescence of bubbles and drops, which present further complexities. The deformation of these bodies can be characterised across six orders of magnitude in length scales, which presents difficulties when studying the dynamic nature of the interaction both experimentally and numerically. Moreover, as a bubble impacts a solid wall, it exerts forces that can remove contaminants or biofilms [77, 83–86]. Menesses et al. [87] have shown that a continuous stream of single bubbles can effectively prevent biofouling by generating consistent shear stress. This principle extends beyond cleaning, influencing the behaviour of bubbles in different mediums and applications. The adhesion behaviour of bubbles or droplets with solids is influenced by the properties of the deformable interface and the surrounding fluid [88], the presence of contaminants [89, 90], and the surface characteristics of the solid, such as its geometry or wettability [91]. As a bubble adheres to a solid surface, it forms a three-phase contact line, which is the interface where the bubble, the solid, and the liquid meet. The dynamics and stability of the contact line are crucial in understanding how bubbles interact with solid surfaces.

In the context of mineral beneficiation, froth flotation is based on bubbles to separate valuable minerals from waste material. The process of flotation depends heavily on the characteristics of the separated particles and the bubbles. Specifically, the surface wettability of the solid particles is crucial for allowing the bubbles to selectively separate hydrophobic from hydrophilic particles [92], and the bubbles must be appropriately sized to enhance the probability of collision between the bubbles and the particles [93]. The main causes behind the detachment of particles from bubbles during flotation separation systems were summarised by Klassen and Mokrousov [94] and Wang et al. [95]. These include the sliding of the particle on the bubble surface, the overall hydrodynamic behaviour of the bubble, such as its lateral migration or deformation, or the collision of the aggregate with a solid wall. When a bubble/particle aggregate collides with a solid horizontal wall, Wang et al. [95] have found that the detachment of the particle depends on the inclination angle of the main axis of the bubble with the solid wall during collision. Comprehensive reviews of recent advances in understanding the hydrodynamics and surface interactions in froth flotation systems can be found in Wang and Liu [96] and Xie et al. [92].

In liquid-solid suspensions, bubbles interact with solid particles, affecting their rise velocity and overall dynamics. Hooshyar et al. [97] have considered the interaction between a rising bubble and a neutrally buoyant particle suspension. The particles were

characterised based on their diameter, and when the size of the particles is sufficiently small, the bubble rises without collision. The work has shown that as the rising bubble interacts with larger particles, the bubble's rise velocity decreases, its surface deforms, and it imparts momentum on the surrounding particles. The bubble will then continue to rise until it interacts with another particle, repeating the cycle of the interaction.

The case of a bubble interacting with a rigid, horizontal wall may be viewed as a special limiting configuration in which the particle size is much larger than the bubble size. The opposite limit is that of a particle crossing an infinitely extended fluid/fluid interface. This configuration has been studied extensively in the context of water entry (air/water interface such that the density ratio is large) by spherical particles [98] and non-spherical particles [99], both in the limit of large impact velocities and in the regime where particles can remain afloat at the fluid/liquid interface [100]. The latter provides an explanation for the phenomenology of water-walking insects. When considering a body translating due to gravity normal to an immiscible interface, certain characteristics of the body's motion and the physical properties of the fluid and the body govern the capability of the body to cross the interface. Given a body in sufficiently slow motion, a static force balance where the weight of the body is greater than the sum of the capillary and buoyancy forces gives an approximate critical condition for breakthrough. The corresponding regime is a flotation regime, or quasi-static detachment regime, as observed by Aristoff and Bush [101] for air/water interfaces and by Pierson and Magnaudet [102, 103] for liquid/liquid interfaces. As inertia becomes more important, shallow or deep seals may form via pinch-off, with the particle entraining a volume of fluid from the upper phase as it settles. For particles crossing a liquid/liquid interface, this regime is often referred to as the tailing regime, and the resulting tails may be axisymmetric or fully three-dimensional. At sufficiently high approach velocities, the three-dimensional tails can also fragment [102]. Although the literature on this topic is extensive, certain configurations, such as the interaction between a bubble and a particle, remain the subject of ongoing development and are not yet as well characterised as the canonical cases [104].

2.6 Summary and remarks

The studies reviewed above show that particle dynamics in homogeneous fluids are now reasonably well understood across a wide range of Reynolds numbers, with clear links between wake structure, path stability and the resulting hydrodynamic forces. Moreover, bubble motion is governed by buoyancy, viscous resistance, inertia and surface tension,

which determine rise speed, deformation and wake development. Depending on the relevant dimensionless groups, bubbles may remain nearly spherical or adopt different shapes, and exhibit wake-driven path instabilities. In stratified fluids, additional mechanisms arise through coupling between buoyancy, diffusion and, where relevant, interfacial stresses, which can alter trajectories and residence times and promote unsteady motion, such as the Marangoni-driven oscillations reported by Li et al. [67].

An important related class of problems concerns a translating body interacting with a horizontal immiscible interface. In the quasi-static limit, breakthrough can be approximated by a static force balance, leading to flotation or quasi-static detachment regimes [101–103]. With increasing inertia, shallow or deep seals may form via pinch-off and the body can entrain upper-phase fluid, yielding a tailing regime for liquid/liquid interfaces that may be axisymmetric or fully three-dimensional, with fragmentation at sufficiently large impact velocities [102].

Overall, while the broader literature on particle and bubble dynamics is extensive, configurations involving the coupled effects of particle geometry and particle-particle interactions in density-stratified fluids, as well as bubble-particle interactions, remain an emerging area and are not yet as well characterised as the canonical single-body problems. These gaps motivate the problems investigated in this thesis.

Chapter 3

Numerical framework

Contents

3.1 Overview	37
3.2 Numerical methods for multiphase flows	37
3.2.1 Key assumptions and conservation equations	37
3.2.2 Numerical methods for deformable interfaces	39
3.2.3 Level-Contour Reconstruction Method (LCRM)	41
3.2.4 Numerical methods for rigid particles	44
3.2.5 Collision modelling	46
3.3 Solving the governing equations	50
3.4 Remarks	59

3.1 Overview

This chapter provides an overview of the numerical methodology employed throughout the thesis. The results presented in the subsequent chapters are obtained from particle-scale direct numerical simulations of particulate flows, both in single-phase configurations and in the presence of a deformable interface. Accordingly, the present chapter describes the governing equations and their discretisation, the approach used to represent and evolve fluid/fluid interfaces, and the numerical treatment of rigid particles and their coupling to the surrounding flow. For completeness, a brief review of alternative modelling and numerical approaches adopted in the literature is also included, in order to place the chosen framework in context.

3.2 Numerical methods for multiphase flows

3.2.1 Key assumptions and conservation equations

In this section, we briefly summarise the modelling assumptions adopted in the direct numerical simulations reported in this thesis. These assumptions are consistent with the Navier-Stokes formulation introduced in Chapter 2 and define the physical regime captured by the numerical framework. In what follows, four modelling assumptions are stated explicitly:

- **Continuum hypothesis.** Both fluid phases are treated as continuous media, such that macroscopic fields are well defined and vary smoothly on the length scales resolved in the simulations.
- **Incompressible Newtonian fluids.** Each phase is modelled as incompressible and Newtonian, with constant viscosity (and, where relevant, constant diffusivity). Where relevant, density variations associated with stratification are assumed small and are retained only in the buoyancy term through the Boussinesq approximation.
- **Sharp boundaries.** Fluid/fluid interfaces are treated as infinitely thin surfaces across which material properties may vary abruptly. Similarly, rigid particles are represented by sharply defined solid boundaries, with fluid/solid coupling enforced through appropriate kinematic and dynamic boundary conditions.

- **Negligible intermolecular forces.** Intermolecular (disjoining) forces are neglected, so that short-range effects such as van der Waals interactions become relevant only at length scales smaller than those resolved here.

Under these assumptions, the incompressible Navier-Stokes equations for the fluid phase may be written as

$$\nabla \cdot \mathbf{u} = 0, \quad (3.1)$$

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right) = \nabla \cdot \mathbf{T} + \mathbf{F}, \quad (3.2)$$

where $\mathbf{T}$ is the (symmetric) stress tensor and $\mathbf{F}$ denotes the gravitational body force term. For an incompressible Newtonian fluid, the stress tensor is given by

$$\mathbf{T} = -p\mathbf{I} + 2\mu\mathbf{S}, \quad (3.3)$$

where $\mathbf{S}$ is the rate-of-deformation tensor, defined as

$$\mathbf{S} = \frac{1}{2} \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T \right), \quad (3.4)$$

and the superscript T denotes the transpose. In the presence of fluid/fluid interfaces and rigid boundaries, Eq. 3.2 must be supplemented by additional force terms to represent surface tension effects and fluid/solid coupling; these contributions are described in detail later.

When considering fluid/fluid interfaces, a set of jump conditions must be imposed so that the velocity field satisfies the Navier-Stokes equations on either side of the interface. Consider a thin control volume that encloses the interface, with unit normal $\mathbf{n}$ and two orthogonal tangential directions defined on the surface. Applying conservation of mass and momentum to this control volume, and assuming that the inward normal mass flux equals the outward normal mass flux (so that there is no accumulation of mass at the interface), leads to the standard interfacial jump conditions:

$$\rho_1 (\mathbf{u}_1 \cdot \mathbf{n} - u_n) - \rho_2 (\mathbf{u}_2 \cdot \mathbf{n} - u_n) = 0, \quad (3.5)$$

where the subscripts 1 and 2 denote quantities evaluated in phases 1 and 2, respectively. Here $\mathbf{n}$ is the unit normal to the interface (taken to point from phase 1 to phase 2), and u_n is the normal velocity of the interface,

$$u_n = \mathbf{u} \cdot \mathbf{n}. \quad (3.6)$$

Furthermore, for incompressible flow in the absence of phase change, the interface is a material surface and the normal velocity is continuous such that:

$$\mathbf{u}_1 \cdot \mathbf{n} = \mathbf{u}_2 \cdot \mathbf{n} = u_n, \quad (3.7)$$

which enforces the no-penetration condition at the interface. In addition, under the assumption of no interfacial slip, the tangential component of the velocity is continuous. For any unit tangent vector $\mathbf{t}$ on the interface,

$$\mathbf{u}_1 \cdot \mathbf{t} = \mathbf{u}_2 \cdot \mathbf{t}. \quad (3.8)$$

Dynamic boundary conditions must also be imposed at the interface. These are obtained from a balance of forces on an interfacial element and may be written as a jump condition for the traction. Denoting the stress tensor in each phase by $\mathbf{T}_i$ ($i = 1, 2$), the interfacial stress balance is

$$(\mathbf{T}_2 - \mathbf{T}_1) \cdot \mathbf{n} = \gamma \kappa \mathbf{n}, \quad (3.9)$$

where γ is the (constant) surface tension and κ is the interface curvature. The surface gradient operator is defined as

$$\nabla_s = (\mathbf{I} - \mathbf{n}\mathbf{n}) \cdot \nabla, \quad (3.10)$$

and the curvature is given by

$$\kappa = -\nabla_s \cdot \mathbf{n}. \quad (3.11)$$

Projecting Eq. 3.9 in the normal direction yields the normal stress balance,

$$\mathbf{n} \cdot (\mathbf{T}_2 - \mathbf{T}_1) \cdot \mathbf{n} = \gamma \kappa, \quad (3.12)$$

while projection onto any unit tangent vector $\mathbf{t}$ on the interface gives the tangential stress condition,

$$\mathbf{t} \cdot (\mathbf{T}_2 - \mathbf{T}_1) \cdot \mathbf{n} = 0. \quad (3.13)$$

3.2.2 Numerical methods for deformable interfaces

When considering multiphase flows, different numerical techniques for interface localisation have been proposed in the literature [105]. In most approaches, the interface is represented by a marker function. These methods are commonly divided into two cat-

egories: interface capturing and interface tracking. Interface capturing methods advect the marker function with the flow, while interface tracking methods explicitly reconstruct and evolve the interface that separates the phases. Below is a brief introduction on the different methods utilised in the literature.

- The volume-of-fluid (VOF) method is one of the most commonly used interface capturing methods. It is based on introducing a colour function C that represents the local volume fraction of one of the phases within each computational cell. By definition, $C = 1$ in cells filled with phase 1, $C = 0$ in cells filled with phase 2, and $0 < C < 1$ in interfacial cells. The evolution of C is obtained by advecting it with the flow field, which allows the interface to be identified as an isosurface of C . The VOF method is commonly described as comprising two main operations: interface reconstruction and interface advection. In the reconstruction step, the distribution of the colour function within a cell and its neighbours is used to infer the position and orientation of the interface. In the widely used piecewise-linear interface calculation (PLIC) approach, the interface is represented locally by a line segment in two dimensions or a plane in three dimensions, with its orientation estimated from nearby volume-fraction values. This reconstruction provides the geometric quantities required by the model, such as the local unit normal and curvature, which are needed to evaluate surface tension forces. After the interface has been reconstructed, the colour function is advanced in time by solving its advection with the given velocity field. This transport step can be performed using geometric schemes, which move the reconstructed interface and update the resulting volume fractions, or using flux-based schemes, which compute phase fluxes across cell faces to update the cell-wise volume fraction. A key advantage of the VOF method is its inherent conservation of mass, since the colour function is evolved as a cell-wise volume fraction through a conservative transport equation. However, the VOF method can suffer from numerical interface smearing, in which the transition region spreads over several cells due to advection errors. In addition, inaccuracies in the reconstruction of curvature and surface tension forcing may generate spurious (parasitic) currents near the interface.
- The level-set method is also widely used for interface capturing. In this approach, the fluid/fluid interface is represented by a continuous level-set function $\phi(\mathbf{x}, t)$, which is typically chosen as a signed-distance function: $\phi > 0$ in one phase, $\phi < 0$ in the other, and $\phi = 0$ on the interface. Advection of the distance function ϕ is

performed by solving the level-set transport equation,

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = 0, \quad (3.14)$$

so that the interface is given by the zero level set, $\phi(\mathbf{x}, t) = 0$. The interface normal and curvature can be obtained directly from ϕ through:

$$\mathbf{n} = \frac{\nabla \phi}{|\nabla \phi|}, \quad \kappa = -\nabla_s \cdot \mathbf{n}. \quad (3.15)$$

In practice, ϕ is often reinitialised to restore its signed-distance property, which improves the accuracy of geometric quantities but may lead to errors in the enclosed volume (and thus mass conservation) if not treated carefully.

- When considering interface tracking methods, the front-tracking method is one of the main approaches used in the literature [105]. In this method, the interface is represented by a set of connected marker points on a Lagrangian mesh, which is advected using the local fluid velocity. The coupling between the Lagrangian interface representation and the underlying Eulerian flow solver is typically achieved through an immersed boundary type framework (IBM), following the approach introduced by Peskin [106] for the numerical study of heart flow. Since the marker points must be explicitly tracked, the method becomes more complex when the interface undergoes severe topological changes, such as interface breakup or coalescence.

In this thesis, a hybrid front-tracking/level-set method is used to represent fluid/fluid interfaces, namely the Level-Contour Reconstruction Method (LCRM) proposed by Shin and Juric [107]. The method and the benefits of this approach are described in Section 3.2.3.

3.2.3 Level-Contour Reconstruction Method (LCRM)

The LCRM provides an interface-tracking framework that avoids the bookkeeping associated with explicitly maintaining and updating marker connectivity, which is typically required in traditional front-tracking methods. The interface is represented on a Lagrangian mesh, using marker points in two-dimensions and triangular surface elements in three dimensions (see Fig. 3.1). A key feature of the method is that the phase surface is treated as a collection of *physically linked* but not *logically connected* elements, so explicit topological connectivity between neighbouring elements does not need to be stored or updated [107]. This locality is advantageous for distributed-memory parallelism,

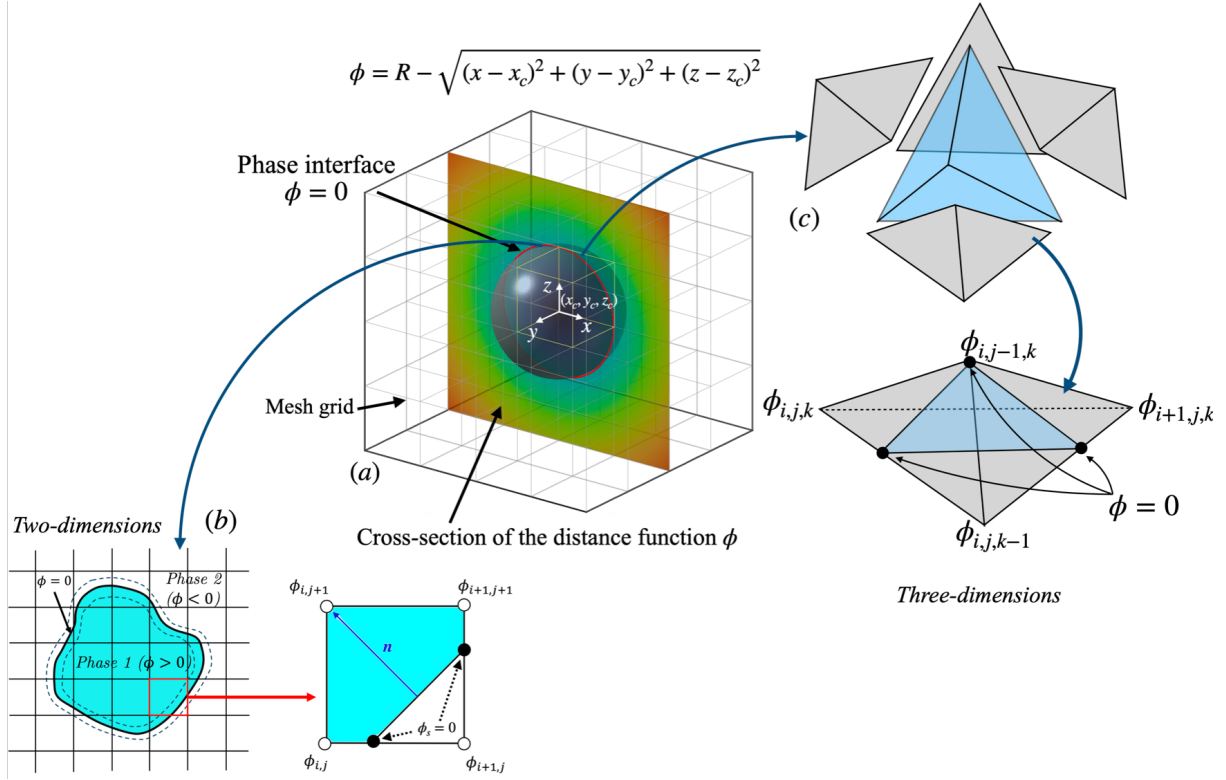


Figure 3.1: Panel (a) shows the three-dimensional Eulerian grid structure with the phase interface, panel (b) presents a schematic of the LCRM in two-dimensions, and panel (c) shows the subdivision of tetrahedral cells in three-dimensions with the tetra-marching procedure for continuous interface interconnection. Figures are adapted from Shin et al. [108].

and Shin et al. [108] demonstrate a parallel LCRM-based solver in which interface operations are performed locally on distributed subdomains. The interface elements are reconstructed as level contours of a characteristic indicator function, which in this thesis is taken to be a Heaviside function, $\mathcal{H}(\mathbf{x}, t)$. For two incompressible immiscible fluids with piecewise-constant properties, the local value of any material property b (such as density or viscosity) can be written as

$$b(\mathbf{x}, t) = b_1 \mathcal{H}(\mathbf{x}, t) + b_2 [1 - \mathcal{H}(\mathbf{x}, t)], \quad (3.16)$$

where the subscripts denote phases 1 and 2, and $\mathcal{H}(\mathbf{x}, t) = 1$ in phase 1 and $\mathcal{H}(\mathbf{x}, t) = 0$ in phase 2.

In the LCRM framework, the Heaviside field can be obtained by solving a Poisson equation [107]:

$$\nabla^2 \mathcal{H}(\mathbf{x}, t) = \nabla \cdot \int_{S(t)} \mathbf{n} \delta(\mathbf{x} - \mathbf{x}_f) \, dS, \quad (3.17)$$

where $\mathbf{x}_f = \mathbf{x}_f(\mathbf{s}, t)$ parametrises the interface $\mathcal{S}(t)$, $\mathbf{n}$ is the unit normal on $\mathcal{S}(t)$, and $\delta(\mathbf{x} - \mathbf{x}_f)$ is the three-dimensional Dirac delta function, which is non-zero only where $\mathbf{x} = \mathbf{x}_f$. Alternatively, $\mathcal{H}$ may be constructed from an Eulerian distance function ϕ , as in level-set methods, which yields an equivalent result [108]. In this case, interface reconstruction in the LCRM is carried out by extracting isocontour surfaces of a scalar signed-distance field within each Eulerian reconstruction cell. In two-dimensions, illustrated in panel (b) of Fig. 3.1, the interface within a cell is represented by a line segment obtained by interpolating the distance values along the cell edges (either with linear interpolation [107] or with higher-order schemes [108, 109]). The interface elements from the previous reconstruction are then discarded, and a new set of elements is generated from the current contour information: the intersection points of the contour with the cell edges define the endpoints of the new elements. Neighbouring cells produce elements that meet at the same physical endpoint locations on shared edges, so the interface is connected implicitly through geometry rather than through stored logical connectivity. The element orientation is chosen consistently so that the associated normal vectors point toward the interior of the region enclosed by the interface.

In three dimensions, illustrated in panel (c) of Fig. 3.1, each Cartesian grid cell is subdivided into five tetrahedral subcells, and the interface is reconstructed within these tetrahedra using the same contour-based procedure as in two-dimensions, applied to the tetrahedral faces. To obtain a globally continuous interface across the domain, the tetrahedra are processed using a consistent marching (tetra-marching) ordering and orientation.

A key benefit of the LCRM is its ability to accommodate complex topological changes without the bookkeeping required in traditional front-tracking. In addition, since the signed-distance field is utilised for reconstruction rather than advected in time, LCRM avoids the mass conservation issues commonly associated with level-set methods. The reconstruction frequency for the work presented in this thesis is set for every 5 time steps (the effect of varying the reconstruction frequency was tested by Shin et al. [110]). The interface is advected in a Lagrangian manner by integrating:

$$\frac{d\mathbf{x}_f}{dt} = \mathbf{V}, \quad (3.18)$$

where $\mathbf{V}$ is the interface velocity. The velocity is obtained by interpolating the Eulerian flow field to the interface and time integration is performed using a second-order Runge-Kutta scheme [108].

3.2.4 Numerical methods for rigid particles

Numerical methods for particle-laden flows are widely reported in the literature, reflecting their prevalence in both natural and industrial settings. These methods do not use any model for the interaction between the fluid and the particle, whereas the fluid flow is governed by the conservation of mass and momentum equations, and the relevant rigid body equations of motion are applied for the solid region, fully resolving the flow field around each particle. Broadly, these methods can be classified into two categories: body-conforming approaches and non-conforming approaches.

For body-conforming methods, the mesh must be updated as particles move, and this often requires repeated remeshing in time, which adds significant computational cost and implementation complexity. In this case, the boundary conditions on the particle surface (described in Chapter 2) are imposed directly on the body-fitted mesh. The main advantage of this approach is an accurate representation of the particle geometry and near-surface flow features, which can improve the prediction of hydrodynamic forces and torques. The main limitation is that maintaining mesh quality becomes increasingly challenging for large particle velocities, close particle/particle or particle/wall interactions, and dense suspensions, where frequent remeshing and additional contact or lubrication treatments may be required.

On the other hand, non-conforming methods enforce the boundary conditions on the particle surface through an additional forcing term in the Navier-Stokes equations. A widely used approach in this class is the immersed boundary method (IBM), in which the presence of the particle is represented on a background Eulerian grid and a body force is introduced to drive the local fluid velocity to the prescribed particle velocity, thereby imposing no slip and no-penetration conditions without requiring a body-fitted mesh. An additional approach is the use of Lagrange multipliers to enforce the boundary conditions (as in Sharma and Patankar [111]). Generally, immersed boundary methods (IBMs) are classified as either continuous forcing or direct (discrete) forcing approaches. In continuous forcing IBMs, the effect of the immersed boundary is represented by a body-force density that is computed from the mismatch between the interpolated fluid velocity at the boundary and the prescribed (desired) boundary velocity. This forcing term is introduced at the continuous level by augmenting the momentum equations prior to discretisation. Continuous forcing is commonly used for problems involving elastic or deformable boundaries (for example Peskin [106]), where the boundary force is obtained from a constitutive law such as Hooke's law and then distributed to the Eulerian grid via a regularised delta function. For rigid boundaries, direct forcing methods are often preferred

in the literature [112]: the IBM force is introduced after discretising the momentum equations, which allows tighter control over the discrete enforcement of the boundary condition and, consequently, the accuracy of the forcing.

The direct forcing immersed boundary method was introduced by Uhlmann [113], in which the fluid and solid equations are advanced sequentially. This procedure is commonly referred to as a weakly coupled approach. First, an intermediate fluid velocity field, $\mathbf{u}^*$, is obtained by solving the Navier-Stokes equations without the immersed boundary forcing associated with rigid particles. The intermediate velocity is then interpolated from the Eulerian grid to the Lagrangian markers on the particle surface. In general, this interpolated velocity differs from the required marker velocity $\mathbf{u}^r$, which follows from the no slip (and no-penetration) condition on the particle boundary. A forcing term is therefore constructed to enforce the constraint,

$$\mathbf{f}_{IBM} = \frac{\mathbf{u}^r - \mathbf{u}^*}{\Delta t}, \quad (3.19)$$

where Δt is the time step. This forcing is then spread back to the Eulerian grid and included in the momentum update to obtain the corrected velocity field. Once the flow has been updated, the hydrodynamic force and torque on each particle can be computed from the immersed boundary forcing and used in the Newton-Euler equations to advance the particle motion. Although popular due to its simplicity, the weakly coupled approach can suffer from stability limitations for light or nearly neutrally buoyant particles; for the method of Uhlmann [113], a lower stability limit of $\rho_p/\rho_f \approx 1.2$ has been reported [105]. Over the years, the original direct forcing scheme of Uhlmann [113] has been extended to strongly coupled formulations to improve stability, particularly for light or nearly neutrally buoyant particles. Developments include a strongly coupled method for spherical particles [114] and a general implicit direct forcing approach for rigid particles of different shapes [115]. A concise summary of these developments is provided by Garcia-Villalba et al. [105].

In this thesis, a fictitious-domain formulation is adopted for the solid particles, with a direct forcing approach used to impose the coupling for the particle region. Related fictitious-domain/direct forcing strategies have been reported in the literature [112, 116–118], and have also been employed in more recent studies [119–121]. In the fictitious-domain method, the particles are initially treated as regions of fluid (often referred to as ‘viscous blobs’) occupying the particle volume on a fixed Eulerian grid. A forcing term is then applied within the particle region to enforce rigid-body motion, so that the particle behaves as a solid, while the flow is still solved on the same background mesh. The main

advantage of this approach is that it accommodates particles of arbitrary shape on a fixed background grid without requiring a body-fitted mesh. Unlike the formulation of Glowinski et al. [122], in which additional equations of motion must be solved to update the rigid-body velocity field $\mathbf{u}_s$, the present approach computes the translational and angular velocities directly from momentum conservation. This avoids solving separate, nonlinear angular-momentum equations and simplifies implementation for bodies with irregular shapes. Since the Eulerian grid remains unchanged, remeshing is avoided and the treatment of large particle displacements and complex particle interactions is simplified. An additional benefit of this approach is that it provides a straightforward framework for treating both fluid/particle interactions and fluid/fluid interfaces within a single solver, such that three-phase flows (two immiscible fluids and a dispersed solid phase) can be simulated without introducing separate numerical frameworks for each interface type. The method utilised in this thesis has been tested for particles in air [123], for which the density ratio is large, and has also been applied to cases with nearly neutrally buoyant particles, as often encountered for microplastics in the ocean. In addition, it has been extended to treat moving contact lines in three-phase flows [124] as well as to incorporate deformable solids [125]. The implementation of the numerical method is summarised in Section 3.3.

3.2.5 Collision modelling

When the interaction between particle pairs or between a particle and a wall is considered, collisions may occur. Accurately modelling these collisions is important for capturing the dynamics of systems with moderate to high particle volume fractions. The collision process typically involves a wide range of length scales, spanning more than two orders of magnitude, which increases the computational difficulty of directly solving all relevant physics [126]. For particle/particle interactions, a thin lubrication layer can form as particles approach, with the fluid in the gap being ‘squeezed’ as the separation decreases. Although adaptive mesh refinement can help resolve this near-contact region, many numerical approaches employ lubrication corrections when the inter-particle gap becomes sufficiently small [41].

Experimental studies have examined collisions between particles and between particles and walls in viscous fluids, such as the work of Gondret et al. [127] (a review of relevant works can be found in Kempe and Fröhlich [126]). These studies show that rebound behaviour, often quantified by the coefficient of restitution, depends mainly on the Stokes impact number $St = \bar{\rho}Re/9$, where $\bar{\rho}$ is again the density ratio between the particle and

the fluid. A critical Stokes number of order $St_c \approx 10$ is typically observed, below which no rebound occurs, while for $St > St_c$ rebound is possible and the restitution coefficient increases with increasing St . Experimental works for particle/particle collisions are more scarce in comparison to particle/wall collisions, largely because of the additional challenges associated with controlling the relative impact conditions and accurately measuring the approach and rebound dynamics of two freely moving particles. As a result, many experimental studies focus on particle/wall configurations, which provide a more repeatable setting for quantifying collision outcomes and validating collision models.

Collision models in the literature are commonly grouped into hard-sphere and soft-sphere approaches. Hard-sphere models treat collisions as quasi-instantaneous events, in which the post-collision velocities are obtained directly from the pre-collision state through an impact law, typically specified in terms of a prescribed coefficient of restitution. These models are typically simpler than soft-sphere models, which resolve collisions over a finite contact time by integrating the particle equations of motion and including contact and dissipative forces during the interaction. Generally, for soft-sphere collision models, very small time steps are required for stability to accurately resolve the collisions. Furthermore, collision models may include both normal and tangential contributions, with the latter accounting for tangential impulse during contact. In many cases, retaining only the normal contribution provides a reasonable approximation for dilute suspensions of smooth, idealised particles, where tangential effects and particle rotation play a secondary role.

In the results presented in this thesis, particle/particle collisions do not play a significant role. The particle volume fractions considered are sufficiently low that close approaches and sustained contacts are rare, and the particle Reynolds numbers are small enough that rebound is unlikely. As a result, the dynamics is dominated by hydrodynamic interactions and particle/fluid coupling. Nonetheless, a simple hard-sphere collision model is implemented, retaining only the normal component and neglecting tangential impulse, to handle the rare cases in which contact occurs. A lubrication correction is also included when the inter-particle gap becomes sufficiently small to account for unresolved near-contact hydrodynamic resistance.

A brief overview of the collision model implemented in the numerical method is presented herein, and an illustration is provided in Fig. 3.2(a). The collision model is a simple impulse response method, where J is the scalar magnitude of the collision impulse. When considering two solid bodies, namely A and B , the linear velocities of these bodies

prior and after collision can be calculated as follows:

$$\mathbf{v}_A^f = \mathbf{v}_A^i - m_A^{-1} J \mathbf{n}, \quad (3.20)$$

$$\mathbf{v}_B^f = \mathbf{v}_B^i + m_B^{-1} J \mathbf{n}, \quad (3.21)$$

where $\mathbf{v}_k^x$ denotes the linear velocity of object $k = (A, B)$ prior to or after collision, denoted by $x = (i, f)$, respectively. Here, m_k denotes the mass of object k .

The angular velocities of the objects may be calculated in a similar manner such that:

$$\boldsymbol{\omega}_A^f = \boldsymbol{\omega}_A^i - J \mathbf{I}_A^{-1} (\mathbf{r}_A \times \mathbf{n}), \quad (3.22)$$

$$\boldsymbol{\omega}_B^f = \boldsymbol{\omega}_B^i + J \mathbf{I}_B^{-1} (\mathbf{r}_B \times \mathbf{n}), \quad (3.23)$$

where $\boldsymbol{\omega}_k^x$ denotes the angular velocity of the object $k = (A, B)$ before or after collision, denoted by $x = (i, f)$, respectively. The inertia tensor is denoted by $\mathbf{I}_k$, and $\mathbf{r}_k$ is the position of the point of collision with respect to the centre of mass of the k^{th} object.

The total velocity of the object at the position of the collision point ($\mathbf{v}_c$) may be calculated as found in Eq. 3.24,

$$\mathbf{v}_{c,k}^x = \mathbf{v}_k^x + \boldsymbol{\omega}_k^x \times \mathbf{r}_k. \quad (3.24)$$

The total velocity of the objects can be used to calculate the relative velocities prior to collision ($\mathbf{v}_r^i$) and after collision ($\mathbf{v}_r^f$) such that ($\mathbf{v}_r^x = \mathbf{v}_{c,B}^x - \mathbf{v}_{c,A}^x$). The coefficient of restitution (e), may be used to relate the relative velocities prior to and after collision, such that:

$$\mathbf{v}_r^f \cdot \mathbf{n} = -e \mathbf{v}_r^i \cdot \mathbf{n}. \quad (3.25)$$

If we substitute these relations into Eq. 3.25, the scalar magnitude of the collision impulse can then be calculated as:

$$J = \frac{-(1+e) \mathbf{v}_r^i \cdot \mathbf{n}}{1/m_A + 1/m_B + (\mathbf{I}_A^{-1} (\mathbf{r}_A \times \mathbf{n}) \times \mathbf{r}_A + \mathbf{I}_B^{-1} (\mathbf{r}_B \times \mathbf{n}) \times \mathbf{r}_B) \cdot \mathbf{n}}. \quad (3.26)$$

Using this collision model, a comparison with the experimental findings of Gondret et al. [127] is presented for the collision of a solid sphere in an ambient fluid with a solid wall. The simulation setup implemented for the validation was similar to that implemented by Biegert et al. [128]. The properties of the ambient fluid and the solid sphere were $\rho_p/\rho_f = 8.34$, $\mu_f = 0.001$ kg/ms, and $D_p = 0.003$ m. The spherical particle was forced to settle in the absence of a gravitational field with a velocity of $u_z(t) = u_{in}(e^{-40t} - 1)$

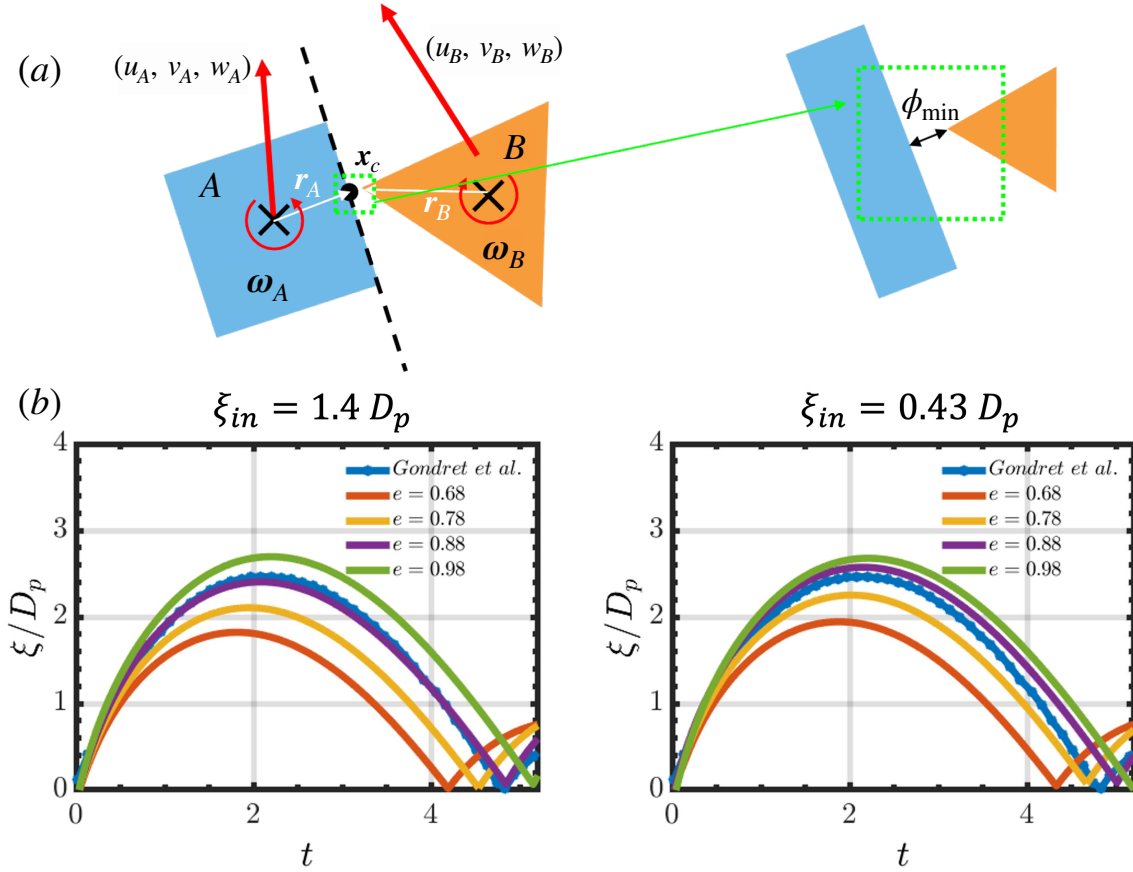


Figure 3.2: Panel (a) shows an illustration of the notation utilised for the collision model. In panel (b), a comparison of the collision model with the experimental results of Gondret et al. [127] for a solid sphere bouncing off a solid wall is provided. Two different initial separation distances were considered, and they are $\xi_{in} = 1.4D_p$ and $\xi_{in} = 0.43D_p$. For these two initial separation distances, four restitution coefficients were tested, ranging between $e = [0.68, 0.98]$.

when the particle was above a specified distance from the solid wall (ξ_{in}). Here, u_{in} is the settling velocity found in the experiment prior to collision. When the distance between the sphere and the solid wall decreased below ξ_{in} , such that $\xi < \xi_{in}$, the forced velocity profile was stopped and the sphere was allowed to settle due to gravity. This is to ensure that the flow field before the collision is similar to that of the experiment. When performing these simulations, $\Delta t_{CFL} = 0.5$ was the controlling time-step (explained in Section 3.3).

Fig. 3.2(b) shows the temporal evolution of the distance between the sphere and the solid wall after the collision when varying ξ_{in} and e . Two different ξ_{in} were considered, and four different coefficients of restitution. When increasing the distance between the particle and the solid wall, the experimental results greatly match the case when $e = 0.88$. Decreasing ξ_{in} leads to the case where the experimental result lies between $e = 0.88$ and $e = 0.78$. Ultimately, the result of the numerical method shows a similar trend to the

experimental result for the evolution of the distance between the sphere and the solid wall post-collision.

For particle-particle collisions, an additional lubrication correction is implemented based on the asymptotic solution of Jeffrey [129]. The normal lubrication model activates if two solid objects are closer than the prescribed distance ($\phi_{cr,max}$):

$$\mathbf{F}_{lub} = \begin{cases} -6\pi\mu R_{cur} (\mathbf{v}_r^i \cdot \mathbf{n}) [\lambda(\phi) - \lambda(\phi_{cr,max})], & \text{if } \phi_{cr,min} \leq \phi_{min} < \phi_{cr,max}, \\ 0, & \text{if } \phi_{min} < \phi_{cr,min} \text{ or } \phi_{min} \geq \phi_{cr,max}. \end{cases} \quad (3.27)$$

If two solid objects are much closer ($\phi_{cr,min}$) then the impulse response model activates. The cut-off separation distance is introduced to ensure that the amplification function remains finite as the separation distance decreases. Here, R_{cur} is the radius of curvature of the solid object. For equally sized spherical particles, the amplification function is

$$\lambda\left(\varepsilon = \frac{\phi}{R_{cur}}\right) = \frac{1}{2\varepsilon} - \frac{9}{20} \ln \varepsilon - \frac{3}{56} \varepsilon \ln \varepsilon, \quad (3.28)$$

where $\varepsilon = \phi/R_{cur}$. Spheres of equal size are assumed, so the signed curvature ratio is $-R_1/R_2 = -1$. For simulations involving more than one particle in the following chapters, the normal coefficient of restitution is set to $e = 0.97$. The lubrication model is activated when the inter-particle gap (surface-to-surface separation) equals one grid cell, and it is deactivated (so that the collision/impulse model takes over) when the gap decreases to 10^{-3} . The choice of $e = 0.97$ corresponds to nearly elastic collisions and is commonly adopted in previous studies [130]. The separation-distance thresholds used to activate and deactivate the lubrication model are similar to those chosen by Ardekani et al. [41].

3.3 Solving the governing equations

The equations governing Newtonian, incompressible multiphase flow are those of mass and momentum conservation. In the present framework, these are written in a single-field formulation that describes the entire system, including both fluid phases and the dispersed solid phase. A smoothed three-dimensional Heaviside function $\mathcal{H}_f(\mathbf{x}, t)$ for the fluid phases is defined as zero in the dispersed fluid phase and unity in the background fluid phase. A similar approach has been used for defining the properties of the solid particle, $\mathcal{H}_s(\mathbf{x}, t)$, which is considered as zero in the solid phase and unity for both fluid phases (the dispersed fluid and the surrounding fluid). The sharp transition between

the phases is resolved numerically with a steep, yet smooth transition across three to four grid cells [108, 131]. In the present implementation, the fluid and solid Heaviside fields are constructed from the signed-distance functions ϕ_f and ϕ_s , respectively. For the fluid/fluid interface, the initial distance field ϕ_f^0 is prescribed on the Eulerian grid from the initial interface geometry. The initial Lagrangian interface elements are then generated from the $\phi_f^0 = 0$ contour. During the simulation, the Lagrangian interface is advected with the interpolated flow velocity, and the Eulerian distance field ϕ_f is subsequently recomputed from the current Lagrangian interface elements by assigning nearby grid points the signed minimum distance to the interface; the sign is determined from the local interface orientation [108, 132]. For the solid phase, ϕ_s is obtained from the particle geometry and updated from the particle position and orientation during the simulation [123]. For a generic distance function ϕ , with $\phi > 0$ in the phase where $\mathcal{H} = 1$, the regularised Heaviside function is evaluated as

$$\mathcal{H}(\phi) = \begin{cases} 0, & \phi \leq -\ell_H, \\ \frac{1}{2} \left[1 + \frac{\phi}{\ell_H} + \frac{1}{\pi} \sin \left(\frac{\pi\phi}{\ell_H} \right) \right], & |\phi| < \ell_H, \\ 1, & \phi \geq \ell_H, \end{cases} \quad (3.29)$$

where $\ell_H = 2\Delta x$ for the uniform Cartesian grid used here, with $\Delta x = \Delta y = \Delta z$. The governing equations may be written as:

$$\nabla \cdot \mathbf{u} = 0, \quad (3.30)$$

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \rho \mathbf{g} + \nabla \cdot (\mu (\nabla \mathbf{u} + \nabla \mathbf{u}^T)) + \mathbf{F} + \mathbf{F}_{FSI}, \quad (3.31)$$

where $\mathbf{u}$, ρ , p , μ , $\mathbf{g}$, $\mathbf{F}$, and $\mathbf{F}_{FSI}$ denote the velocity, density, pressure, viscosity, gravitational acceleration, the local surface tension force at the interface, and the direct forcing term for fluid-structure interaction, respectively. A hybrid formulation for the surface tension force is employed [108, 110]:

$$\mathbf{F} = \gamma \kappa_{H_f} \nabla \mathcal{H}_f. \quad (3.32)$$

Again, γ is the surface tension, considered constant, and κ_{H_f} is twice the mean interface curvature calculated on the Eulerian grid using the following equations,

$$\kappa_{H_f} = \frac{\mathbf{F}_L \cdot \mathbf{N}}{\gamma \mathbf{N} \cdot \mathbf{N}}, \quad (3.33)$$

$$\mathbf{F}_L = \int_{\mathcal{S}(t)} \gamma \kappa_f \mathbf{n}_f \delta_f(\mathbf{x} - \mathbf{x}_f) dS, \quad (3.34)$$

$$\mathbf{N} = \int_{\mathcal{S}(t)} \mathbf{n}_f \delta_f(\mathbf{x} - \mathbf{x}_f) dS. \quad (3.35)$$

In Eqs. 3.34–3.35, following from Section 3.2.3, $\mathbf{x}_f$ is a parameterisation of the interface, $\mathcal{S}(t)$, and $\delta_f(\mathbf{x} - \mathbf{x}_f)$ is a three-dimensional Dirac delta function that is non-zero only at the interface. Furthermore, $\mathbf{n}_f$ is the unit normal vector to the interface, where the interface has an area element, dS ; κ_f is again twice the mean interface curvature, however, it is now obtained from the Lagrangian interface structure [108, 131]. The geometric information in $\mathbf{N}$, such as the unit normal $\mathbf{n}_f$ and the interface infinitesimal area dS , is directly computed from the Lagrangian interface, then distributed onto the Eulerian grid using a discrete delta function [106]. Interface advection follows from 3.18. Further details on calculating the force, constructing the function field $\mathbf{N}$ and the Heaviside function, and advecting the interface can be found in [109, 110, 132–135].

The particle’s motion and interaction with the fluid are modeled using a fictitious domain method, such that the Navier-Stokes equations are applied to the entire flow field. Tracking the solid body’s motion is achieved by introducing a distance function ϕ_s . At the start of the simulation, ϕ_s^0 is analytically calculated at the cell centre of the Eulerian grid (x_i^0, y_i^0, z_i^0) to create the solid volume, which is then updated to calculate ϕ_s^n at (x_i^n, y_i^n, z_i^n) by tracking the solid’s centre position and rotation over time. The solid object’s movement is updated by its momentum averaged translational and rotational velocities, which are calculated in Eqs. 3.36 and 3.37:

$$m_p \mathbf{u}_p = \int_{\mathcal{V}} \rho \mathbf{u} dV, \quad (3.36)$$

$$\mathbf{I}_p \boldsymbol{\omega}_p = \int_{\mathcal{V}} \mathbf{r} \times \rho \mathbf{u} dV, \quad (3.37)$$

where m_p is the mass of the solid, $\mathbf{u}_p$ is its translational velocity, $\mathcal{V}$ is the solid volume, $\mathbf{r}$ is the radial vector from its centre, $\mathbf{I}_p$ is the moment of inertia, and $\boldsymbol{\omega}_p$ is the rotational velocity. The moment of inertia can be calculated using Eq. 3.38,

$$\mathbf{I}_p = \int_{\mathcal{V}} \rho_p |(\mathbf{r} \cdot \mathbf{r}) \mathbf{I} - \mathbf{r} \otimes \mathbf{r}| dV, \quad (3.38)$$

and the position of the solid can be tracked by the following velocity field:

$$\mathbf{u}_s(x, y, z) = \mathbf{u}_p + \boldsymbol{\omega}_p \times \mathbf{r}. \quad (3.39)$$

The centroid position $\mathbf{x}_p$ of the particle is updated as described in Eq. 3.40:

$$\frac{d\mathbf{x}_p}{dt} = \mathbf{u}_s. \quad (3.40)$$

This procedure is efficient compared to fluid/fluid interface tracking since only centroid position as well as angular rotation of the solid object are traced. Similar to the method used for the interface advection, the time integration is performed using a second-order Runge-Kutta scheme [123].

Rigid-body constraints are enforced within the solid region to ensure zero deformation. In this approach, the solid region is treated as a fluid, but an additional forcing term is introduced to maintain rigidity. A high viscosity coefficient is assigned to the solid region, and the velocity field is updated everywhere in the computational domain following the same procedure as in an all-fluid simulation. As a result, the computed velocity inside the solid region is typically not equivalent to the centroid translational and rotational velocities obtained from Eqs. 3.36 and 3.37. The momentum-averaged translational and rotational velocities are computed, and the forcing term is subsequently used to correct the solid velocity toward the required rigid-body field, such that:

$$\mathbf{F}_{FSI} = \rho \frac{\mathbf{u}_s - \mathbf{u}}{\Delta t}, \quad (3.41)$$

where the corresponding rigid-body velocity field is prescribed as $\mathbf{u}_s(\mathbf{x}, t)$ (Eq. 3.39). If the assigned artificial solid viscosity is sufficiently high, the correction applied over a time step becomes very small. In practice, a viscosity about 100 times that of the fluid is sufficient [123]; in this work, a solid viscosity 500 times the fluid viscosity is utilised. The role of the artificial solid viscosity was tested by Mirzaii and Passandideh-Fard [136]. In the fictitious domain method, $\mathbf{F}_{FSI}$ is used not only to match the velocity at the particle surface, but also to make sure the rigid particle accelerates correctly. Because of this, the tentative particle velocity is not known in advance and must be solved together with the fluid equations. The rigid-body equation of motion is enforced implicitly through the coupled fluid equations [117]. Different methods have been developed over time, see for instance [117, 136, 137]. The present framework is similar to the method adapted by Mirzaii and Passandideh-Fard [136] and Lu et al. [138].

Within the single-fluid formulation, the material properties in the domain are calculated as follows

$$\rho(\mathbf{x}, t) = [\rho_b + (\rho_l - \rho_b)\mathcal{H}_f(\mathbf{x}, t)] \mathcal{H}_s(\mathbf{x}, t) + \rho_p(1 - \mathcal{H}_s(\mathbf{x}, t)), \quad (3.42)$$

$$\mu(\mathbf{x}, t) = [\mu_b + (\mu_l - \mu_b)\mathcal{H}_f(\mathbf{x}, t)]\mathcal{H}_s(\mathbf{x}, t) + \mu_p(1 - \mathcal{H}_s(\mathbf{x}, t)), \quad (3.43)$$

where the subscripts (l, b, p) denote the background fluid, the dispersed fluid, and the solid phase, respectively.

The code is implemented in Fortran 2008, and consists of two main modules: (i) one for solving the incompressible Navier-Stokes equations, and (ii) for interface tracking and reconstructing the interface. For parallelisation, an algebraic domain decomposition technique is utilised, such that communication across adjacent subdomains is managed via Message passing interface (MPI) protocol. The numerical procedure follows the LCRM-FDM framework used by Yoon et al. [123]. In the present work, the same single-field formulation is solved on a fixed three-dimensional Cartesian Eulerian grid. The procedure can be separated into an initialisation stage and a time-integration loop:

(i) Initialisation

1. The computational domain is generated on a fixed Cartesian Eulerian grid. The initial velocity and pressure fields are prescribed.
2. The fluid/fluid and solid/fluid interfaces are initialised using the distance functions ϕ_f and ϕ_s , respectively. The Heaviside fields $\mathcal{H}_f$ and $\mathcal{H}_s$ are then constructed, and the corresponding density and viscosity fields are evaluated.
3. Where a fluid/fluid interface is present, the initial Lagrangian interface elements are generated from the $\phi_f = 0$ contour on the underlying Eulerian grid.

(ii) Time integration

1. At each time step, the material properties are updated from the current Heaviside fields ($\mathcal{H}_f$ and $\mathcal{H}_s$).
2. Where a fluid/fluid interface is present, the LCRM is used to evaluate the interface geometry and surface-tension force.
3. The Navier-Stokes equations are solved over the full domain, with the solid treated as a moving fictitious-domain region. A pressure projection is then applied to enforce incompressibility.
4. The particle translational and angular velocities are obtained from the momentum inside the solid volume, and the rigid-body velocity is imposed through $\mathbf{F}_{FSI}$.

5. The particle position and orientation are advanced, and the solid distance function ϕ_s and Heaviside field $\mathcal{H}_s$ are updated.
6. The fluid/fluid interface is advected, and where applicable, the Lagrangian interface elements are reconstructed from ϕ_f for the next time step.
7. Contact-line, lubrication, and collision models are applied only in cases where the corresponding near-contact interaction occurs.

The incompressible Navier-Stokes equations, Eq. 3.31, are advanced in time using Chorin's projection method [139]. In this fractional-step approach, the non-pressure terms are first used to obtain an intermediate velocity field, after which a pressure correction is computed to enforce the incompressibility constraint. Spatial discretisation is performed on a staggered Marker-and-Cell (MAC) grid [140], with scalar quantities stored at cell centres, and velocity components stored at cell faces. The nonlinear convective term is discretised using a second-order essentially non-oscillatory (ENO) scheme [141, 142], while the remaining terms are approximated using second-order centred finite differences. In the implementation, the ENO face values are obtained by selecting the upwind stencil from the sign of the face velocity and applying a local slope correction based on the smaller-magnitude neighbouring one-sided difference. No explicit flux-corrected transport limiter is used. The time integration is split into two sub-steps. For clarity, the fractional-step procedure is written below in first-order form; in the simulations reported in this thesis, the same projection framework is advanced using the second-order temporal scheme described later in this section. Extension to a second-order accurate scheme can be straightforwardly achieved by performing two successive first-order steps and then averaging the velocities at t^n and t^{n+2} ($\mathbf{u}^n$ and $\mathbf{u}^{n+2}$) [143].

The discrete form of the momentum equation can be written as:

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} = \frac{1}{\rho^{n+1}} (\mathbf{A}_h^n + \mathbf{F}_h^n) - \frac{1}{\rho^{n+1}} \nabla_h p, \quad (3.44)$$

where $\mathbf{A}_h^n$ denotes the convective, diffusive, and gravitational terms, $\mathbf{F}_h^n$ incorporates the surface tension force and the FSI force, and the subscript h refers to a spatially discrete operator. Note that the FSI force at this point is zero, such that the solid region is treated as a fluid. First, an intermediate velocity $\mathbf{u}^*$ is introduced, where the effect of pressure is not considered:

$$\frac{\mathbf{u}^* - \mathbf{u}^n}{\Delta t} = \frac{1}{\rho^{n+1}} (\mathbf{A}_h^n + \mathbf{F}_h^n), \quad (3.45)$$

and second, the final divergence-free velocity $\mathbf{u}^{n+1}$ is obtained via the pressure projection:

$$\mathbf{u}^{n+1} = \mathbf{u}^* - \frac{\Delta t}{\rho^{n+1}} \nabla_h p. \quad (3.46)$$

By enforcing $\nabla_h \cdot \mathbf{u}^{n+1} = 0$ one obtains the pressure Poisson equation

$$\nabla_h \cdot \left(\frac{1}{\rho^{n+1}} \nabla_h p \right) = \frac{\nabla_h \cdot \mathbf{u}^*}{\Delta t}, \quad (3.47)$$

which is solved using the hybrid multigrid/GMRES iterative method described below.

For the solid/fluid interaction, the FSI force is computed using a fast-fictitious domain approach. The divergence-free velocity field $\mathbf{u}^{n+1}$ does not in general satisfy the rigidity constraint inside the solid region. The rigid-body translational and angular velocities, $\mathbf{u}_p^{n+1}$ and $\boldsymbol{\omega}_p^{n+1}$, are obtained by conserving linear and angular momentum in the solid domain $\mathcal{V}$:

$$m_p \mathbf{u}_p^{n+1} = \int_{\mathcal{V}} \rho_p \mathbf{u}^{n+1} dV, \quad (3.48)$$

$$\mathbf{I}_p \boldsymbol{\omega}_p^{n+1} = \int_{\mathcal{V}} \mathbf{r} \times (\rho_p \mathbf{u}^{n+1}) dV. \quad (3.49)$$

The rigid-body velocity field inside the solid is then:

$$\mathbf{u}_s^{n+1} = \mathbf{u}_p^{n+1} + \boldsymbol{\omega}_p^{n+1} \times \mathbf{r}. \quad (3.50)$$

Imposing rigidity in $\mathcal{V}$ is equivalent to applying an FSI forcing term inside the solid region, defined at the next time step as [144]:

$$\mathbf{F}_{FSI}^{n+1} = \frac{\rho_p}{\Delta t} (\mathbf{u}_s^{n+1} - \mathbf{u}^{n+1}), \quad (3.51)$$

where $\mathbf{u}^{n+1}$ is the solenoidal velocity predicted by the solver (viz. Eq. 3.46) prior to enforcing rigid-body motion in the solid region. If particle collisions are detected during the time step, the particle velocities are updated accordingly before the rigid-body constraint is imposed. As seen by Fadlun et al. [116], different procedures can be used to assign the solid velocity at grid points near the immersed boundary. In the *stepwise* approach, the forcing is applied at the grid points closest to the boundary, treating the boundary as if it passes through those points, so no interpolation is performed and the geometry is represented in a stepwise manner; the surface is also effectively smeared because the three velocity components are enforced at slightly different locations. In the *weighted volume-fraction* approach, for each cell cut by the boundary, the fraction of the cell occupied by the solid is computed and used as a weight to scale the forcing applied

to the unknowns closest to the boundary. In the *velocity-interpolation* approach, rather than scaling the forcing, an effective imposed velocity is first estimated at the nearest grid point (under a linear assumption) so that it is consistent with the boundary moving with the solid velocity, and the forcing is then applied using this effective velocity. Although the velocity-interpolation procedure is generally more accurate for flows at high Reynolds numbers, all three approaches typically give comparable results under moderate Reynolds numbers [116]. In that regime, it is therefore reasonable to favour the least expensive option computationally, since the added cost of the more accurate procedure is unlikely to yield a noticeable improvement in the solution.

The BLUE solver allows several temporal discretisations, including Euler, Crank–Nicolson, and Gear schemes. In the simulations reported in this thesis, the projection framework is advanced using a second-order Gear scheme, with implicit treatment of the viscous terms. A Generalised Minimal Residual (GMRES) iterative solver is used to solve for the viscous contributions to the velocity field, such that the discontinuous viscosity coefficients appear in the solver’s linear operator in the usual manner. In contrast, discontinuities in the density field complicate the pressure Poisson equation: they lead to a non-separable operator, which is particularly challenging to handle efficiently in parallel implementations. Consequently, a hybrid multigrid/GMRES algorithm is employed to solve the pressure based on the work of Kwak and Lee [145], which is well suited for large density contrasts [108]. The multigrid procedure can be outlined as follows. First, a second-order, cell-centred finite-difference discretisation of Eq. 3.47 is constructed. The discontinuous coefficient ($1/\rho$) is then treated using a harmonic averaging scheme. During grid coarsening, the residual is transferred to coarser levels using linear interpolation. In the prolongation step, the error correction is interpolated back to finer grids in a manner that preserves cell fluxes on the coarse levels. Relaxation of the linear system on the fine grids is carried out using a parallel red-black successive over-relaxation (SOR) method. Finally, the error on the coarsest grid is solved using a parallel GMRES algorithm. Additional details for the implementation can be found in Shin et al. [108]. The time-step, Δt , at each temporal iteration is set to satisfy the following criterion:

$$\Delta t = \min\{\Delta t_{cap}, \Delta t_{CFL}, \Delta t_{int}, \Delta t_{vis}\}, \quad (3.52)$$

where Δt_{cap} , Δt_{CFL} , Δt_{int} , Δt_{vis} are the capillary, Courant-Friedrichs-Lewy (CFL), interfacial, and viscous time-steps, respectively. These time-steps are defined as follows, where

$\Delta x_{\min} = \min_j(\Delta x_j)$ is the minimum size x for cell j :

$$\begin{aligned}\Delta t_{cap} &\equiv \frac{1}{2} \sqrt{\frac{(\rho_b + \rho_l) \Delta x_{\min}^3}{\pi \gamma}}, & \Delta t_{CFL} &\equiv \min_j \left(\min_{\text{domain}} \left(\frac{\Delta x_j}{u_j} \right) \right), \\ \Delta t_{int} &\equiv \min_j \left(\min_{\Gamma(t)} \left(\frac{\Delta x_j}{\|\mathbf{V}\|} \right) \right), & \Delta t_{vis} &\equiv \min \left(\frac{\rho_b}{\mu_b}, \frac{\rho_l}{\mu_l} \right) \frac{\Delta x_{\min}^2}{6}.\end{aligned}\tag{3.53}$$

At each time step, information must be transferred between the moving Lagrangian interface and the stationary Eulerian grid. Since the interface marker locations $\mathbf{x}_f^m$ do not, in general, coincide with the Eulerian grid points $\mathbf{x}_{ij}$, Peskin's IBM [106] is employed. In this approach, the infinitely thin interface is represented by a smooth distribution function that spreads interfacial source terms over 3–4 grid points near the interface. In the same manner, field variables are interpolated from the Eulerian grid to the interface. Because the (numerical) interface thickness, of order the grid size, is kept fixed throughout the simulation, no numerical diffusion is introduced [107].

To illustrate the procedure in two dimensions, interfacial source contributions may be written in the form

$$\Phi = \int_{\mathcal{S}(t)} \psi \delta(\mathbf{x} - \mathbf{x}_f) dS, \tag{3.54}$$

where ψ is a generic interfacial source term and $\mathbf{x}_f$ denotes a point on the interface $\mathcal{S}(t)$. For an interface marker m , ψ^m is located at $\mathbf{x}_f^m = (x_f^m, y_f^m)$. Consider a discrete Eulerian field variable R_{ij} defined on a uniform grid with $\Delta \mathbf{x} = (\Delta x, \Delta y)$. Approximating the Dirac delta function by the smooth IBM distribution function $D_{i,j}$, spreading of ψ^m to the Eulerian grid is performed as

$$\Phi_{i,j} = \sum_m \psi^m D_{i,j}(\mathbf{x}_f^m) \Delta S, \tag{3.55}$$

where ΔS is the interface element length associated with marker m . Conversely, interpolation of R_{ij} from the Eulerian grid to marker m is given by

$$R_f^m = \sum_{i,j} R_{i,j} w_{i,j}^m = \sum_{i,j} R_{i,j} D_{i,j}(\mathbf{x}_f^m) \Delta x \Delta y, \tag{3.56}$$

where $w_{i,j}^m = D_{i,j}(\mathbf{x}_f^m) \Delta x \Delta y$ are the interpolation weights. These weights satisfy $\sum_{i,j} w_{i,j}^m = 1$, ensuring R_f^m is bounded by the surrounding grid values.

Following Peskin and McQueen [146], the distribution function is defined as

$$D_{i,j}(\mathbf{x}_f^m) = \frac{d(r_x)d(r_y)}{\Delta x \Delta y}, \quad r_x = \left(\frac{x_f^m}{\Delta x}\right) - i, \quad r_y = \left(\frac{y_f^m}{\Delta y}\right) - j, \quad (3.57)$$

with the one-dimensional kernel $d(r)$ given by

$$d(r) = \begin{cases} d_1(r), & |r| \leq 1, \\ \frac{1}{2} - d_1(2 - |r|), & 1 < |r| < 2, \\ 0, & |r| \geq 2, \end{cases} \quad (3.58)$$

where

$$d_1(r) = \frac{3 - 2|r| + \sqrt{1 + 4|r| - 4r^2}}{8}. \quad (3.59)$$

The extension to three dimensions can be implemented in a straightforward manner by defining $D_{i,j,k} = d(r_x)d(r_y)d(r_z)/(\Delta x \Delta y \Delta z)$ and using the appropriate surface element in (3.55).

3.4 Remarks

This chapter has presented the numerical framework used throughout the thesis. The numerical methods adopted for multiphase flows were described first, including key assumptions and implementation details in the present framework and brief comparisons with alternative formulations in the literature. These assumptions also define the limitations of the simulations. The calculations resolve particle-scale flows in finite computational domains whose dimensions are typically several particle diameters and do not impose background turbulence or large-scale environmental circulation. The achievable Schmidt number and density-interface thickness are therefore constrained by the grid resolution required to resolve the near-surface scalar boundary layers. Furthermore, the fictitious domain method was introduced for the treatment of rigid particles, followed by the collision model used to handle near-contact interactions; its validation was also presented. All simulations reported in this thesis were performed on high-performance computing facilities provided by the Imperial College London Research Computing Service.

Chapter 4

On the motion of a particle in a density-stratified fluid

Contents

4.1	Introduction	61
4.1.1	Non-dimensional equations	62
4.2	Benchmark tests	65
4.3	Simulation Setup	69
4.4	Results and discussion	70
4.4.1	Rising disc dynamics in a homogeneous ambient	71
4.4.2	Rising disc dynamics in a density-stratified ambient	77
4.5	Concluding remarks	90

Related manuscript: *A. M. Abdal*, D. Panda, L. Kahouadji, M. Shams, S. Shin, J. Chergui, D. Juric, and O. K. Matar. ‘Numerical simulations of annular disc dynamics in homogeneous and density-stratified fluids at moderate Reynolds number’. *Under revision, Phys Rev Fluids*.

4.1 Introduction

The rise and settling dynamics of isolated particles in density-stratified fluids is central to many environmental and geophysical transport processes, where stable density gradients arise from variations in temperature or salinity. In such settings, even the motion of a single rigid particle can differ markedly from that in a homogeneous ambient, with stratification modifying the transient dynamics and the approach to a steady settling or rising speed, and in sufficiently strong stratification leading to pronounced unsteady behaviour such as oscillations or prolonged residence near a density transition layer [14, 15, 30, 54]. Since a detailed discussion of prior work is provided in the literature review chapter, the focus here is restricted to the modelling framework, validation, and the subsequent application to isolated non spherical particles.

Consider an incompressible Newtonian fluid with a stable background stratification and adopt a fictitious domain, one fluid formulation under the Boussinesq approximation. The flow is governed by the continuity equation and the momentum equation, written in dimensional form as:

$$\nabla \cdot \mathbf{u} = 0, \quad (4.1)$$

$$\rho_0(\mathbf{x}, t) \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \nabla \cdot [\mu(\mathbf{x}, t) (\nabla \mathbf{u} + \nabla \mathbf{u}^T)] + \rho(\mathbf{x}, t) \mathbf{g} + \mathbf{F}_{FSI}, \quad (4.2)$$

where $\mathbf{u}$ is the velocity, p is the pressure, and $\mathbf{g}$ is the gravitational acceleration. The indicator function $\mathcal{H}_p(\mathbf{x}, t)$ is equal to 1 within the particle and 0 in the surrounding fluid. In this one fluid setting, the reference density on the left hand side of Eq. 4.2 is defined as:

$$\rho_0(\mathbf{x}, t) = \rho_{f,0} (1 - \mathcal{H}_p(\mathbf{x}, t)) + \rho_p \mathcal{H}_p(\mathbf{x}, t). \quad (4.3)$$

In the body force term, the density field ρ is defined as:

$$\rho(\mathbf{x}, t) = \rho_f(\mathbf{x}, t) (1 - \mathcal{H}_p(\mathbf{x}, t)) + \rho_p \mathcal{H}_p(\mathbf{x}, t). \quad (4.4)$$

Similarly, the dynamic viscosity field is given by

$$\mu(\mathbf{x}, t) = \mu_f (1 - \mathcal{H}_p(\mathbf{x}, t)) + \mu_p \mathcal{H}_p(\mathbf{x}, t), \quad (4.5)$$

where $\rho_{f,0}$ is a reference fluid density, $\rho_f(\mathbf{x}, t)$ is the local fluid density, ρ_p is the particle density, μ_f is the fluid dynamic viscosity, and μ_p is the viscosity assigned within the particle region in the fictitious domain formulation. The evolution of the stratification is

modelled through a transport equation for the density field:

$$\frac{\partial \rho_f}{\partial t} + \mathbf{u} \cdot \nabla \rho_f = \kappa \nabla^2 \rho_f, \quad (4.6)$$

where κ is the molecular diffusivity of the stratifying agent. Within the fictitious domain formulation described in Chapter 3, the fluid equations are solved over the entire domain while the particle region is constrained to follow rigid body motion. The transport equation is also solved on the same domain, with the scalar diffusivity set to zero inside the rigid particle region, so that the particle is treated as impermeable to the stratifying agent [30, 35].

In the homogeneous limit, the fluid density and viscosity are uniform, so the one fluid formulation reduces to the incompressible Navier–Stokes equations with constant material properties. These validation tests quantify the ability of the solver to reproduce established particle velocity histories and reference terminal speeds across a range of Reynolds numbers and stratification strengths. After establishing this baseline accuracy for spheres, we turn to non-spherical particles. In many applications, particles rarely possess idealised spherical shapes, and their geometry can strongly influence the hydrodynamic forces and the resulting rise or settling dynamics. Motivated by this, we consider a disc-shaped particle with finite permeability, modelled here through a central aperture.

The remainder of this chapter first introduces the non-dimensional formulation adopted in this thesis, then validates the numerical implementation using benchmark cases of spherical particles settling in homogeneous and stratified fluids, before presenting the corresponding results for rising annular discs in a density-stratified fluid with emphasis on how density-stratification and the presence of a central perforation modify the observed dynamics.

4.1.1 Non-dimensional equations

To non-dimensionalise the governing equations, we introduce the following scalings for the spatial coordinate $\mathbf{x}$, velocity $\mathbf{u}$, time t , pressure p , and fluid density ρ_f :

$$\tilde{\mathbf{x}} = \frac{\mathbf{x}}{R_{eq}}, \quad \tilde{\mathbf{u}} = \frac{\mathbf{u}}{U}, \quad \tilde{t} = \frac{t}{R_{eq}/U}, \quad \tilde{p} = \frac{p}{\rho_{f,0} U^2}, \quad \tilde{\rho}_f = \frac{\rho_f - \rho_{f,0}}{\gamma R_{eq}}, \quad (4.7)$$

where tildes denote dimensionless variables. Here, $R_{eq} = ((3/16)h[D_D^2 - d^2])^{1/3}$ is the equivalent radius of a sphere having the same volume as the disc, where D_D is the outer

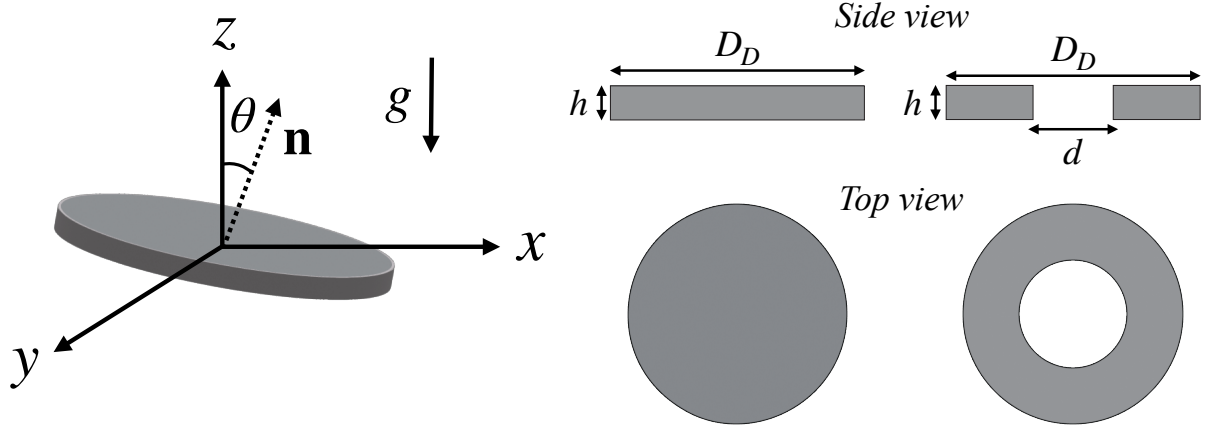


Figure 4.1: Schematic of the disc geometry. The coordinate system, gravity direction, and inclination angle θ between the disc normal $\mathbf{n}$ and the vertical z axis are shown. Side and top views compare a solid disc and a perforated disc of outer diameter D_D and thickness h , with a central hole of diameter d .

disc diameter, d is the diameter of the annulus, and h is the disc thickness, which is governed by the aspect ratio $\chi = D_D/h$ (see Fig. 4.1). The characteristic gravitational velocity scale is defined as

$$U = \sqrt{R_{eq}|\hat{\rho}|g}, \quad (4.8)$$

where $\hat{\rho}$, which is expressed by

$$\hat{\rho} = \frac{\rho_{f,0} - \rho_p}{\rho_{f,0}} > 0, \quad (4.9)$$

is the (positive) relative density contrast between the reference fluid density $\rho_{f,0}$, taken at the initial disc position z_0 , and the disc density ρ_p . In this work, $\hat{\rho} \approx 0.01$ is kept constant in all cases, similar to the experiments of Fernandes et al. [19]. This choice of $\hat{\rho}$ is representative of microplastics in the ocean, for which the particle density is often close to that of the surrounding seawater [3]. The unperturbed background fluid density profile is assumed linear,

$$\rho_f(z) = \rho_{f,0} + \gamma z, \quad (4.10)$$

with $\gamma = d\rho_f/dz < 0$ the constant density gradient within the computational domain.

The corresponding dimensionless mixture density (excluding the stratification contribution) is then:

$$\tilde{\rho}_0 = (1 - \mathcal{H}_p) + \frac{\rho_p}{\rho_{f,0}} \mathcal{H}_p = 1 - |\hat{\rho}| \mathcal{H}_p. \quad (4.11)$$

Using the above scalings, the non-dimensional governing equations read

$$\tilde{\nabla} \cdot \tilde{\mathbf{u}} = 0, \quad (4.12)$$

$$\tilde{\rho}_0 \frac{D\tilde{\mathbf{u}}}{D\tilde{t}} = -\tilde{\nabla}\tilde{p} + \frac{1}{Ar} \tilde{\nabla} \cdot (\tilde{\nabla}\tilde{\mathbf{u}} + \tilde{\nabla}\tilde{\mathbf{u}}^T) + \mathcal{H}_p \mathbf{e}_z + \frac{1}{Fr^2} \tilde{\rho}_f (1 - \mathcal{H}_p) \mathbf{e}_z + \tilde{\mathbf{F}}_{FSI}, \quad (4.13)$$

$$\frac{D\tilde{\rho}_f}{D\tilde{t}} = \frac{1}{Ar Sc} \tilde{\nabla}^2 \tilde{\rho}_f, \quad (4.14)$$

where $D/D\tilde{t} = \partial/\partial\tilde{t} + \tilde{\mathbf{u}} \cdot \tilde{\nabla}$ is the material derivative, $\mathbf{e}_z$ is the unit vector in the vertical direction, and $\tilde{\mathbf{F}}_{FSI}$ denotes the non-dimensional fluid-structure interaction force, implemented using a direct forcing method [116] to impose the rigid-body velocity field inside the solid region. The hydrostatic pressure component $-Re_q g \mathbf{e}_z / U^2$ is incorporated within the pressure gradient term.

The dimensionless groups that appear in Eqs. (4.12)–(4.14) are the Archimedes, Froude and Schmidt numbers, defined as:

$$Ar = \frac{Re_q U \rho_{f,0}}{\mu_f}, \quad Fr = \frac{U}{N Re_q}, \quad Sc = \frac{\mu_f}{\rho_{f,0} \kappa}, \quad (4.15)$$

where N is the buoyancy frequency defined by:

$$N^2 = -\frac{g}{\rho_{f,0}} \gamma. \quad (4.16)$$

The Archimedes number is utilised rather than the Reynolds number as the rising velocity of the disc is not known *a priori*, and the Reynolds number herein is defined as $Re = \sqrt{D_D^2 - d^2} V_t \rho_{f,0} / \mu_f$ where V_t is the terminal velocity as determined from the simulations.

In non-dimensional form, using $\rho_{f,0}$ and μ_f as reference scales for density and viscosity, the mixture density and viscosity fields are:

$$\tilde{\rho}(\tilde{\mathbf{x}}, \tilde{t}) = \frac{\rho_f(\mathbf{x}, t)}{\rho_{f,0}} [1 - \mathcal{H}_p(\tilde{\mathbf{x}}, \tilde{t})] + \frac{\rho_p}{\rho_{f,0}} \mathcal{H}_p(\tilde{\mathbf{x}}, \tilde{t}), \quad (4.17)$$

$$\tilde{\mu}(\tilde{\mathbf{x}}, \tilde{t}) = [1 - \mathcal{H}_p(\tilde{\mathbf{x}}, \tilde{t})] + \frac{\mu_p}{\mu_f} \mathcal{H}_p(\tilde{\mathbf{x}}, \tilde{t}). \quad (4.18)$$

Table 4.1: Simulation setup utilised for the homogeneous fluid benchmark cases.

Case	Domain size ($L_x \times L_y \times L_z$)	Mesh size	D_p (mm)	ρ_p (kg/m ³)	μ_f (kg/(m · s))	ρ_f (kg/m ³)	Re
1	$0.15 \times 0.15 \times 0.2$	$256 \times 256 \times 384$	15	1120	0.113	960	11.6
2	$0.15 \times 0.15 \times 0.2$	$256 \times 256 \times 384$	15	1120	0.058	960	31.9
3	$0.01 \times 0.01 \times 0.03$	$384 \times 384 \times 1152$	0.5	2560	9.03×10^{-4}	1000	41.0

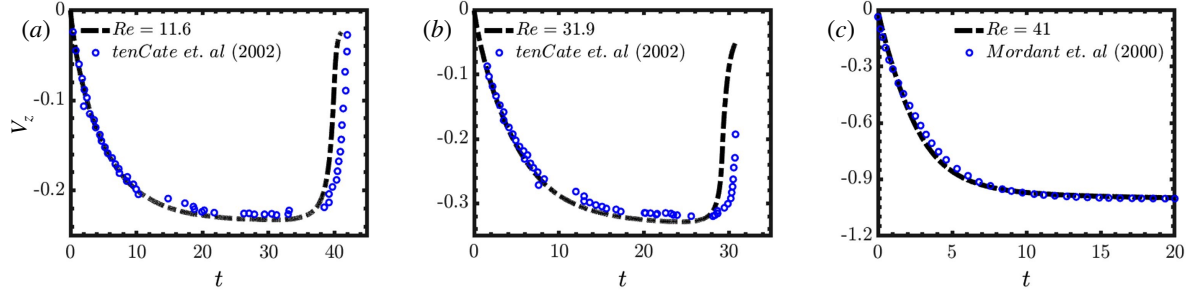


Figure 4.2: Validation of the numerical technique: comparison of the temporal evolution of the particle settling velocity in a homogeneous fluid obtained from numerical method and published experimental data; (a) and (b), and (c) show results for $Re = 11.6$ and 31.9 [147], and $Re = 41$ [148], respectively.

4.2 Benchmark tests

To validate the numerical implementation in a homogeneous fluid configuration, two experimental studies of spherical particle settling that span different Reynolds numbers were considered [147, 148]. The corresponding simulation parameters are summarised in table 4.1 and closely follow the setups adopted by Yao et al. [149]. Because the settling dynamics is dictated by the coupled fluid and particle properties, the terminal velocity was not known *a priori*. Therefore, the Reynolds number, $Re = LU/\nu$, was evaluated using terminal velocity measurements reported in the experiments, and L is taken as the spherical particle diameter D_p . In this chapter, the domain boundary conditions are periodic on the lateral boundaries, while the top and bottom boundaries satisfy free-slip and no-penetration conditions. For the pressure projection, a Neumann condition is used for the pressure at the top and bottom boundaries. Since the pressure is therefore determined only up to an arbitrary additive constant, the pressure gauge is fixed internally in the solver [150].

For the cases at $Re = 11.6$ and $Re = 31.9$ [147], the computed velocity histories are consistent with those reported in the literature as seen in panels (a) and (b) of Fig. 4.2. In these simulations, the spherical particle is released from rest at an initial position of 0.13 m. In the plots, time is normalised by the gravitational time scale $\sqrt{D_p/g}$ and velocity is normalised by the gravitational velocity scale $\sqrt{D_p g}$. The particle exhibits an initial acceleration phase followed by an approach to an approximately constant settling speed. In the present finite domain, the particle eventually reaches the bottom boundary, after which the velocity magnitude decreases to zero as the particle comes to rest at the bottom of the container.

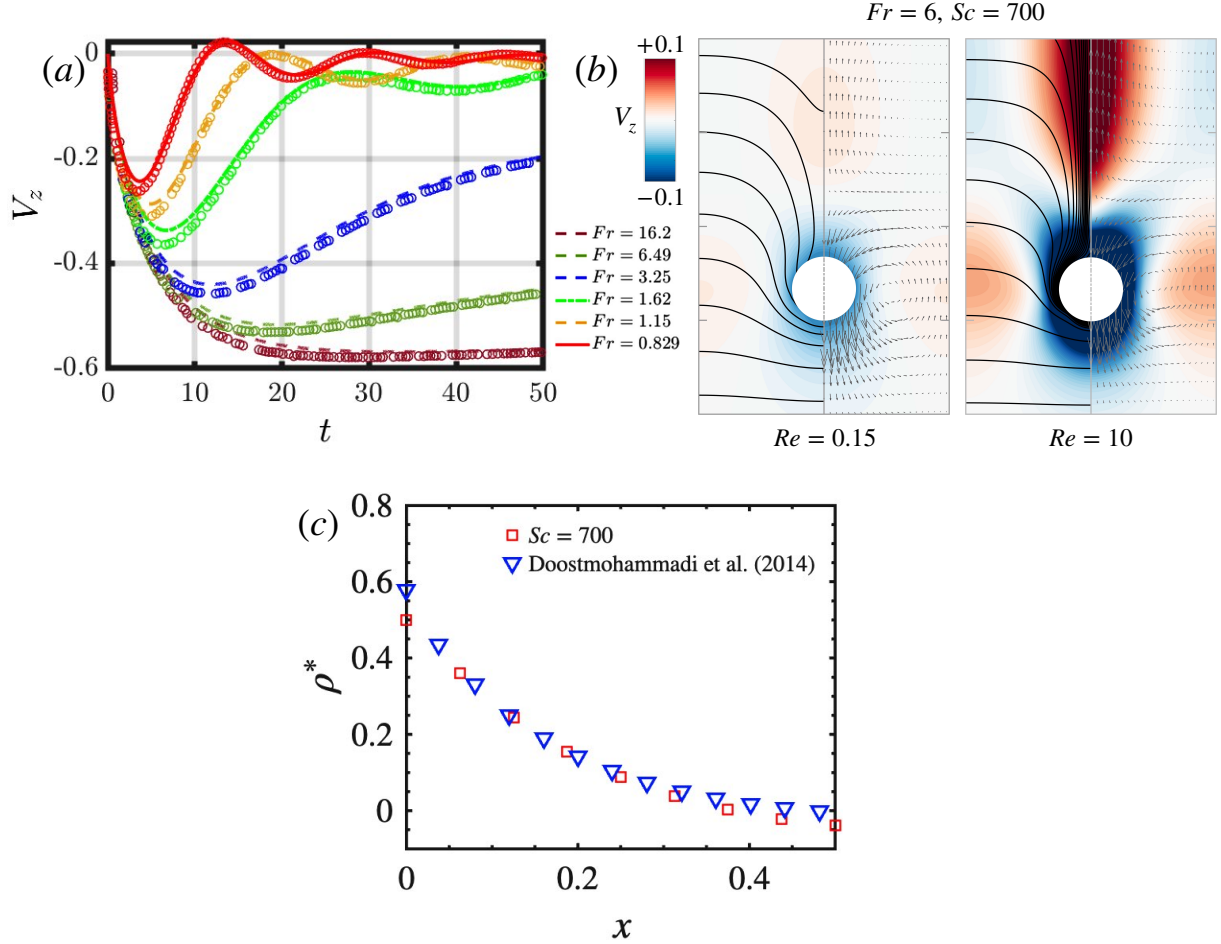


Figure 4.3: Panel (a) presents a comparison with the results of Doostmohammadi et al. [30] (markers) for a sphere settling in a linearly stratified fluid with $Re = \rho_{f,0}U_s D_p / \mu_f = 14.1$ and different Fr , where U_s is the Stokes settling velocity. Panel (b) shows the corresponding flow field for a spherical particle settling in a linearly stratified fluid at fixed $Sc = 700$ and $Fr = 6$, for two Reynolds numbers, $Re = 0.15$ and $Re = 10$. The left subpanels show the isopycnals, while the right subpanels show glyphs of the velocity field. Panel (c) shows the variation of the dimensionless perturbed density $\rho^* = (\rho_f - \rho_f|_{z=z_{\text{peak}}})/(\gamma D_p)$ along the horizontal $z = z_{\text{peak}}$ plane near the sphere at peak particle velocity for $Re = 14.1$, $Fr = 1.62$, $Sc = 700$.

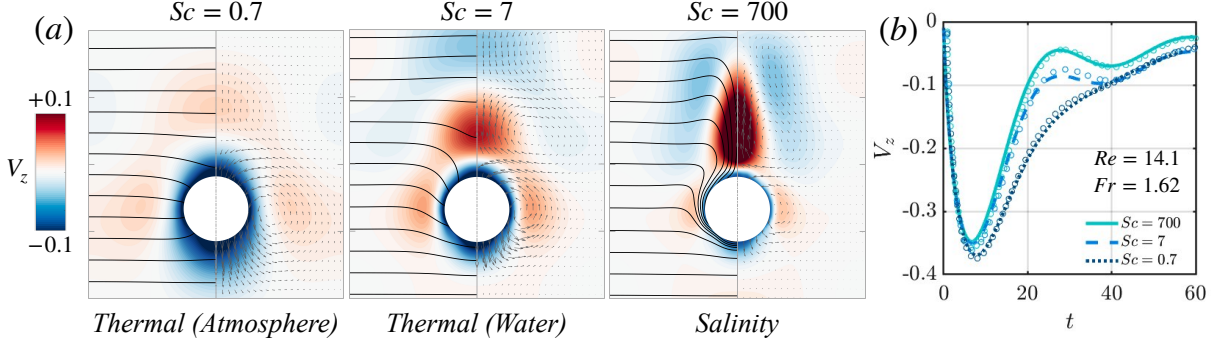


Figure 4.4: Panel (a) presents sample flow fields in the vicinity of a settling sphere in a linearly stratified fluid as the Schmidt number Sc is varied, with $Re = \rho_{f,0}U_s D_p / \mu_f = 14.1$ and $Fr = 1.62$, where U_s denotes the Stokes settling velocity. Panel (b) shows the corresponding particle velocity profiles for these cases, compared with the results of Doostmohammadi et al. [30] (markers).

A small discrepancy is observed for both Reynolds numbers, where the predicted terminal velocity magnitude is slightly larger than the reference data. As a result, the particle reaches the bottom boundary marginally earlier than in the reported results. For the case at $Re \approx 41$ [148] provided in panel (c) of Fig. 4.2, simulations were performed using a spatial resolution of approximately $D_p / \Delta x \approx 20$. The computed velocity profiles show good agreement with the experimental measurements, with a root mean squared error (RMSE) below 3%. These benchmark tests in a homogeneous fluid demonstrate that the numerical framework employed in this thesis accurately captures the settling dynamics observed in the experiments.

Furthermore, we validate the numerical framework against Doostmohammadi et al. [30] for the settling of a rigid sphere in a linearly stratified fluid (panel (a) of Fig. 4.3). The computational domain is $12D_p \times 12D_p \times 24D_p$, with the particle initially placed $2D_p$ below the top boundary; the reference fluid density $\rho_{f,0}$ is evaluated at the initial particle location and used to define the particle Reynolds number and the Froude number ($Fr = U/(NL)$). Following Doostmohammadi et al. [30], the characteristic velocity is taken as the Stokes terminal velocity, $U_s = (\rho_p - \rho_{f,0})gD_p^2/(18\mu_f)$, and in Fig. 4.3(a) we hold $(Re, Sc) = (14.1, 700)$ fixed while varying Fr across multiple cases. The resulting settling velocity profiles show excellent agreement with Doostmohammadi et al. [30]; while the near-surface boundary layer may not be fully resolved on the present grids, resolution tests with $D_p / \Delta x = 20$ and $D_p / \Delta x = 32$ yield an RMSE below 1% between the two, consistent with the minimal sensitivity reported by Doostmohammadi et al. [30] when varying the resolution from $D_p / \Delta x = 12.5$ to $D_p / \Delta x = 50$. Overall, these comparisons provide confidence in the accuracy and reliability of the proposed computational approach, both in the weakly density-stratified regime and in the strongly stratified regime, where

the particle eventually reaches a level at which the local fluid density matches the particle density. Additionally, panel (b) presents two representative simulations illustrating the effect of varying Re while holding Fr and Sc constant. For $Re = 0.15$, the isopycnals (solid black contours in the left panel) exhibit only weak distortion, and the caudal wake is characterised by a weak vertical velocity directed opposite to the settling motion. In contrast, at $Re = 10$ the isopycnals are substantially displaced, accompanied by the emergence of a pronounced jet in the wake with markedly enhanced upward velocity. In panel (c), the variation of the dimensionless perturbed density $\rho^* = (\rho_f - \rho_f|_{z=z_{\text{peak}}})/(\gamma D_p)$ along the horizontal $z = z_{\text{peak}}$ plane near the sphere at peak particle velocity is compared to the results obtained by Doostmohammadi et al. [30] when $Re = 14.1$, $Fr = 1.62$, $Sc = 700$. The figure shows that the shape of the isopycnals is similar to that reported by Doostmohammadi et al. [30], with the density perturbation decaying monotonically away from the particle surface along the horizontal plane.

Additional tests of the numerical method are presented in Fig. 4.4. Here, $Re = 14.1$ and $Fr = 1.62$ are fixed while the Schmidt number is varied; panel (a) shows the corresponding flow field in the particle vicinity and panel (b) presents the time history of the settling velocity, compared with the results of Doostmohammadi et al. [30]. Varying Sc has a non-trivial effect on the local density field, with a larger volume of lighter fluid displaced by the particle as Sc increases. The impact on the settling velocity profile is more modest, however, as the peak velocity magnitude remains similar across the cases. Finally, as discussed in Chapter 2, the oscillations in the vertical velocity are associated with the generation of internal waves, an effect that becomes more pronounced at larger Sc , as seen in panel (b).

In summary, the benchmark tests show that the present numerical framework reproduces the main trends reported in the reference studies for both homogeneous and density-stratified fluids across a range of stratification strengths. In a linearly stratified fluid, the predicted settling histories and flow structures are in excellent agreement with Doostmohammadi et al. [30], and the simulations capture the coupled response of the velocity and density fields, including internal-wave signatures that become more pronounced at larger Sc . With this validation established, we now turn to the setup adopted for the dynamics of impervious and annular discs.

4.3 Simulation Setup

We solve the governing equations in a three-dimensional Cartesian box of size $L_x \times L_y \times L_z = 9D_D \times 9D_D \times 48D_D$. The domain is decomposed into parallel subdomains, each covered by a uniform 64^3 finite-difference grid. The global mesh therefore contains $384 \times 384 \times 2048$ points, corresponding to a spatial resolution of $D_D/\Delta x = 42.67$. This resolution was verified to be sufficient to resolve both the disc rising velocity and the transient jet structures. The global mesh contains approximately 3.02×10^8 grid points and is decomposed into 1152 parallel subdomains. A representative disc simulation was advanced for $\mathcal{O}(10^4)$ time steps using 1152 parallel processes distributed over 18 CPU compute nodes, and required approximately four days of wall-clock time.

In this work, we consider a disc aspect ratio $\chi = 7$, unless otherwise stated. This aspect ratio is chosen to be similar to previous works on rising and settling discs in homogeneous and stratified fluids [19, 37]. When considering the transient dynamics of rising or settling rigid and annular discs, it is convenient to introduce the non-dimensional moment of inertia I^* [151]:

$$I^* = \frac{1}{64} \frac{\rho_p}{\rho_{f,0}} \pi \frac{h}{D_D} \left(1 - \frac{d^4}{D_D^4} + \frac{4}{3} \frac{h^2}{D_D^2} \left(1 - \frac{d^2}{D_D^2} \right) \right), \quad (4.19)$$

which characterises the resistance of the disc to rotation about its centroid. One possible strategy for comparing rigid and annular discs is to enforce the same value of I^* between configurations, in addition to fixing the Archimedes and Froude numbers. This would, however, generally require adjusting the disc aspect ratio $\chi = D_D/h$, which may have a nontrivial influence on the hydrodynamic response for moderately thick discs [20]. In the present work, we therefore adopt a different approach: for a given aspect ratio, we fix the total mass of the disc and vary D_D when switching between rigid and annular geometries, so that removing material from the centre does not change the overall mass. With this choice, the corresponding variation in I^* remains modest; when d/D_D is varied from 0 to 0.5, I^* changes by less than 7%, which we consider acceptable for the comparisons reported below [22].

In addition, it is important to ensure that the near-surface flow is adequately resolved in our simulations. In a stratified fluid, a density boundary layer develops together with the velocity boundary layer as discussed in Chapter 2. Resolving the near-surface density boundary layer is essential because it controls the local density gradients close to the particle surface, and hence the stratification-induced forces and torques acting on the particle. If this layer is under-resolved, the near-surface gradients may not be captured

accurately, leading to inaccurate predictions of the particle motion; by analogy, for heated or cooled bodies, an under-resolved thermal boundary layer would give inaccurate surface heat fluxes and buoyancy-driven flow. Classical boundary layer theory predicts that its thickness scales as $\delta_\rho \sim \mathcal{O}(1/\sqrt{Re Sc})$; however, this estimate may not be directly applicable to the moderate Reynolds numbers considered here [30]. Torres et al. [32] indicate that, at moderate Reynolds numbers, the density boundary layer can be up to four times thicker than this classical estimate. Moreover, at intermediate Froude and Reynolds numbers, Inman et al. [27] reported a scaling of the form $\delta_\rho \sim \mathcal{O}(1/(Re Sc)^{1/3})$. Motivated by these observations, and in order to ensure adequate resolution of the density boundary layer for all configurations considered, we set the Schmidt number to $Sc = 0.7$ or $Sc = 7$, following More et al. [35]. These values are representative of a thermally-stratified atmosphere and of water, respectively. With this choice, the density boundary layer is resolved by at least a few grid points across the range of Reynolds and Froude numbers examined in this study.

Lastly, in this work, the disc is released from a vertical position of $2D_D$ from the bottom of the domain, with an initial inclination $\theta_0 = 5^\circ$, where θ is defined in Fig. 4.1. Previous studies have typically adopted similar initial angles, $\theta_0 \in [0^\circ, 10^\circ]$ [37, 152]. Nevertheless, previous work indicates that the long-term particle motion is independent of initial inclination, both in homogeneous conditions [153] and in a density-stratified environment [37]. Lastly, both rising and falling particles are relevant in oceanic stratified flows, depending on the particle density relative to the surrounding seawater. The present study focuses on rising particles, which is directly relevant to buoyant microplastics, while falling particles are more representative of dense or biofouled particles. Although the direction of motion changes the sign of the density contrast encountered by the particle, the underlying stratification-induced effects on the wake, hydrodynamic forces, and particle migration remain closely related.

4.4 Results and discussion

The following sections present simulation results for discs rising in (i) a homogeneous fluid and (ii) a density-stratified fluid, with the objective of isolating the influence of a central perforation on the disc dynamics. We examine how the perforation modifies key features of the motion, including the rise velocity, trajectory and inclination angle, and the associated wake structure relative to an impervious disc. Throughout, the trends observed in the simulations are compared against relevant experimental and numerical

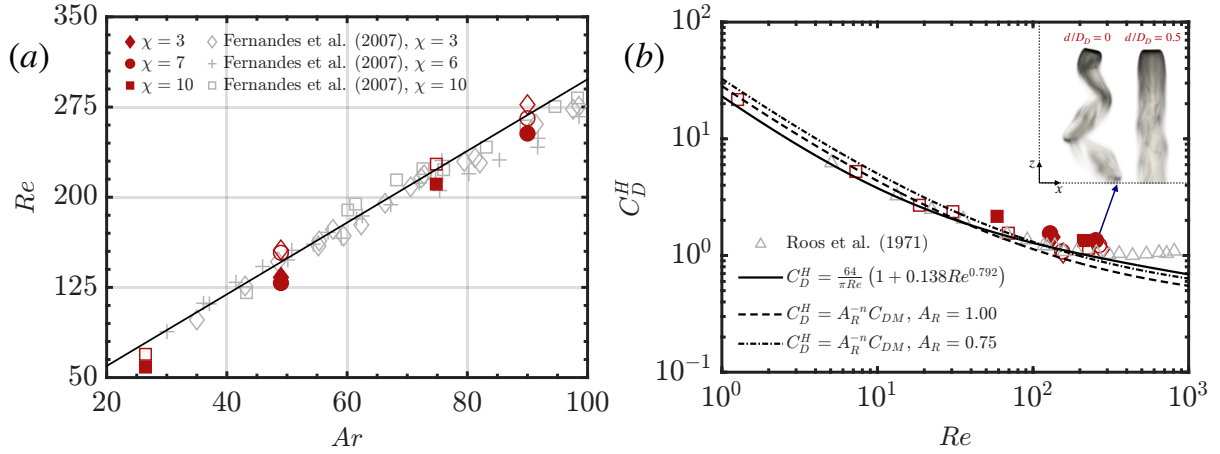


Figure 4.5: Panel (a) shows the Reynolds number against the Archimedes number for rising discs in a homogeneous fluid. The computational results are presented against the experimental results of Fernandes et al. [154] for various aspect ratios χ . The solid line corresponds to $C_D^H = 1.2$. Panel (b) compares the drag coefficient C_D^H from the simulations to empirical correlations and experimental measurements [155]. The inset shows two sample volume renderings of the vorticity profile for an impervious and perforated disc with $d/D_D = 0.5$ ($Ar = 90$, $\chi = 7$). The unfilled red markers correspond to the simulation results with solid discs, and the filled red markers correspond to perforated discs with $d/D_D = 0.5$.

results available in the literature to place the present findings in context and to validate the observed computational results.

4.4.1 Rising disc dynamics in a homogeneous ambient

We start the discussion of the results by drawing comparisons between our numerical results and the experiments of Fernandes et al. [19] for unperforated discs. Fig. 4.5 presents the variation of the Reynolds numbers, calculated from the mean rising velocity after the discs have reached steady state behaviour in a homogeneous fluid, with the Archimedes number. The unfilled markers in Fig. 4.5 correspond to unperforated discs, whereas filled markers correspond to perforated discs with $d/D_D = 0.5$. The plots include simulation results for varying disc aspect ratios (χ), ranging between $\chi = 3$ and $\chi = 10$.

The slope obtained from the data plotted in Fig. 4.5(a) is typically used to determine the drag coefficient (C_D^H) of rising or settling objects. In a homogeneous fluid, the drag coefficient can be extracted under the assumption of steady state behaviour, after the disc has reached a terminal velocity. In steady state, the sum of all forces acting parallel to

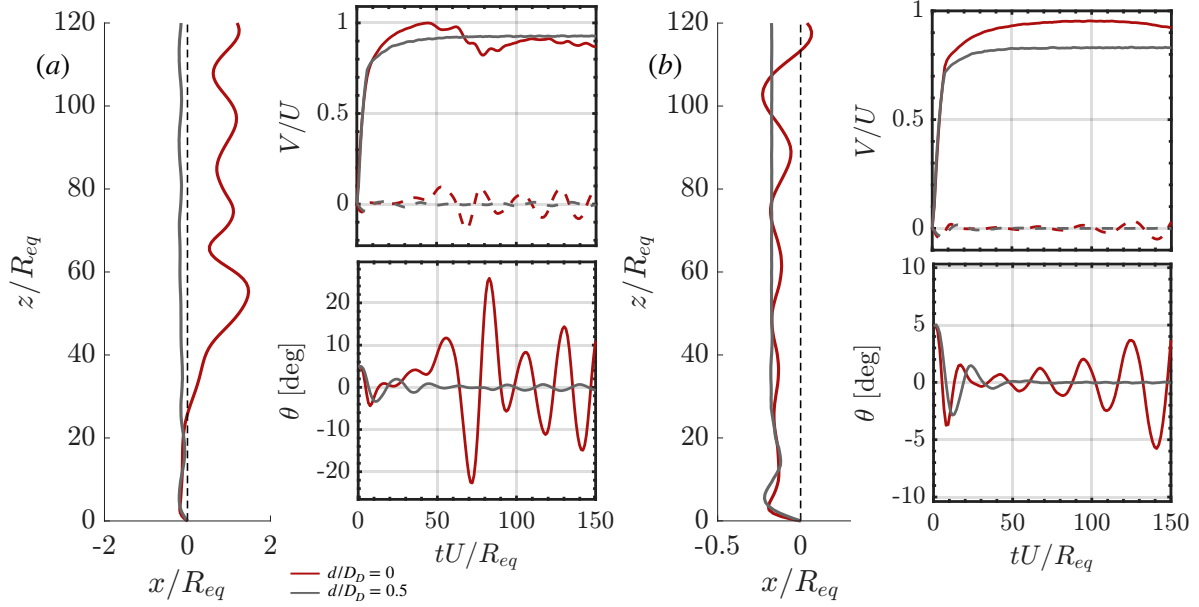


Figure 4.6: Disc trajectory in the x - z plane (side view), time histories of the vertical (V_z , solid) and lateral (V_x , dashed) velocities, and the inclination angle θ shown for $Ar = 90$, $\chi = 7$, and $Ar = 49$, $\chi = 7$ in (a) and (b), respectively. Here, $I^* = 0.0072$ for solid discs, and $I^* = 0.0067$ for perforated discs.

the vertical direction is balanced by the buoyancy force (F_B), which is constant in time for a homogeneous fluid. Assuming rising or settling with a broadside-on orientation, this balance gives [156]:

$$(\rho_{f,0} - \rho_p)g\mathcal{V} = \frac{1}{2}\rho_{f,0}C_D^H V_t^2 A_s, \quad (4.20)$$

where $\mathcal{V} = \pi(D_D^2 - d^2)h/4$ is the volume of the disc and $A_s = \pi(D_D^2 - d^2)/4$ is the solid area. The drag coefficient can then be readily extracted as $C_D^H = 2|\hat{\rho}|hg/V_t^2$. To relate Eq. 4.20 to Fig. 4.5, the Archimedes number may be rewritten as

$$Ar = \sqrt{\frac{3}{16} \frac{\rho_{f,0} \sqrt{gh} |\hat{\rho}| \sqrt{D_D^2 - d^2}}{\mu_f}}. \quad (4.21)$$

From the definitions of the Reynolds and Archimedes numbers and Eq. 4.20, it follows that C_D^H can be expressed in terms of Re and Ar as:

$$C_D^H = \frac{32}{3} \frac{Ar^2}{Re^2}. \quad (4.22)$$

Physically, the dependence of C_D^H on Ar^2/Re^2 arises because Ar characterises the buoyancy forcing, while Re characterises the resulting rise velocity, so their ratio measures the drag required to balance the buoyancy-driven motion [19]. In Fig. 4.5(a), the solid line

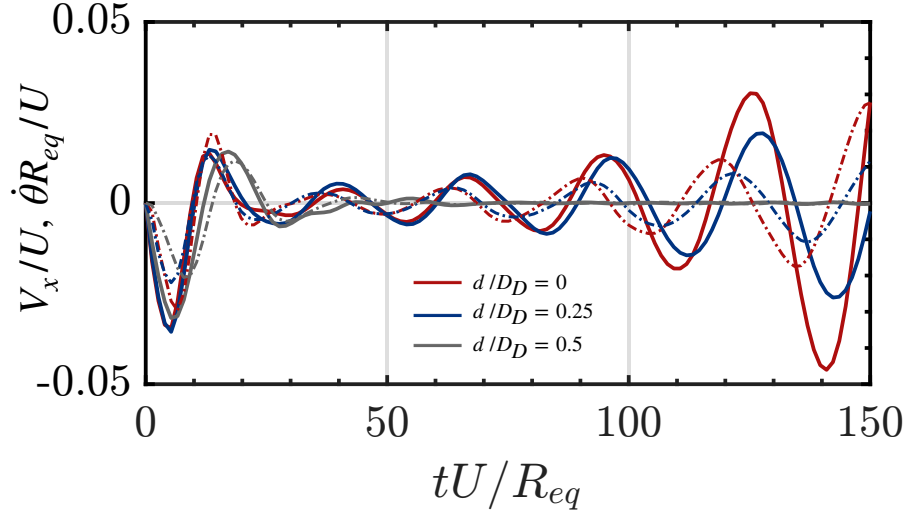


Figure 4.7: Time histories of the disc lateral velocity V_x (solid lines) and angular velocity $\dot{\theta}$ (dash-dotted lines) for $Ar = 49$ and $\chi = 7$, with varying d/D_D . The corresponding dimensionless moments of inertia are $I^* = [0.0072, 0.0071, 0.0067]$ for $d/D_D = [0, 0.25, 0.5]$, respectively.

represents the prediction obtained using a constant drag coefficient ($C_D^H = 1.2$), and it compares favourably with the experimental measurements of Fernandes et al. [19]. The numerical results for the unperforated discs are consistent with this trend, whereas the perforated discs yield systematically lower Re at a given Ar (with no discernible dependence on χ), indicating a modest increase in the effective drag due to the presence of the perforation. A similar increase in the drag coefficient was found when comparing the flow around dandelion seeds with impervious discs [157], attributed to the reduced projected area of the former. Furthermore, the dependence of C_D^H on χ contrasts with the behaviour reported for rising spheroids at high Reynolds numbers by Will et al. [18], who found that C_D^H increases from approximately 0.59 for a sphere to about 2.08 for an oblate spheroid with a small aspect ratio.

Fig. 4.5(b) compares the numerical predictions of the drag coefficient, C_D^H , as a function of the Reynolds number, Re , with two empirical correlations and experimental measurements from Roos and Willmarth [155]. Additionally, two sample volume renderings of the vorticity profile are provided in the inset for $Ar = 90$, $\chi = 7$. The first correlation,

$$C_D^H = \frac{64}{\pi Re} (1 + 0.138 Re^{0.792}), \quad (4.23)$$

is applicable to discs with $\chi > 1$ settling or rising broadside-on for $1.5 \lesssim Re \lesssim 130$ [37, 158]. We also consider a formulation developed for ice particles falling in air that

accounts for the projected area ratio (A_R) [156, 159],

$$A_R = \frac{A_s}{A}, \quad A = \frac{\pi D_D^2}{4}, \quad C_D^H = A_R^{-n} C_{DM}, \quad (4.24)$$

where

$$C_{DM} = C_0 \left(1 + \frac{\delta_0}{Re^{1/2}} \right)^2. \quad (4.25)$$

Here, $n = \frac{1}{2}$, $C_0 = 0.35$, and $\delta_0 = 8$, following Heymsfield and Westbrook [159]. This formulation was also adopted by Tinklenberg et al. [156] in their analysis of the settling dynamics of solid and perforated discs in quiescent and turbulent air. Although originally developed for ice particles falling in air, its relevance here is therefore geometric rather than regime-specific. In general, both correlations provide reasonable estimates of C_D^H at low Re ; however, they slightly underestimate C_D^H as Re increases. The numerical results for solid discs are in excellent agreement with the measurements of Roos and Willmarth [155] over the range of Re considered.

Fig. 4.6 shows four representative simulation cases: (a) $Ar = 90$, $\chi = 7$ and (b) $Ar = 49$, $\chi = 7$, each for a solid disc and a perforated disc with $d/D_D = 0.5$. The corresponding moment of inertia for the solid and perforated cases are $I^* = 0.0072$ and $I^* = 0.0067$, respectively. When the discs are released from rest with a finite initial inclination angle ($\theta_0 = 5^\circ$), they rotate to a broadside-on orientation ($\theta = 0^\circ$) as they align to maximise the projected area normal to the direction of motion. After this initial reorientation, the side view trajectories in the $x/R_{eq}-z/R_{eq}$ plane indicate that the solid discs undergo a pronounced fluttering motion during ascent for both Ar considered. Furthermore, the time histories of the vertical (V_z) and lateral (V_x) velocities are shown (solid and dashed lines, respectively). For the solid disc at $Ar = 90$, the vertical velocity V_z exhibits weak oscillations once the initial transient associated with the disc's acceleration from rest has ended [19].

The fluttering regime is further characterised by oscillations of the disc's inclination angle. From the frequency f of these pitching oscillations, we define the Strouhal number based on the disc diameter D_D and the terminal velocity V_t as $St = fD_D/V_t$. For the solid discs, we obtain $St = 0.17$ at $Ar = 90$ and $St = 0.13$ at $Ar = 49$, which is similar to previous works [19, 20]. Introducing a central perforation suppresses the fluttering dynamics: the perforated discs rise along a nearly rectilinear trajectory with negligible lateral drift. This behaviour is observed for both $Ar = 90$ and $Ar = 49$, as indicated by the near-zero lateral velocity V_x and the markedly reduced oscillations of the inclination angle θ after the initial transient. In addition, once the perforated discs attain their

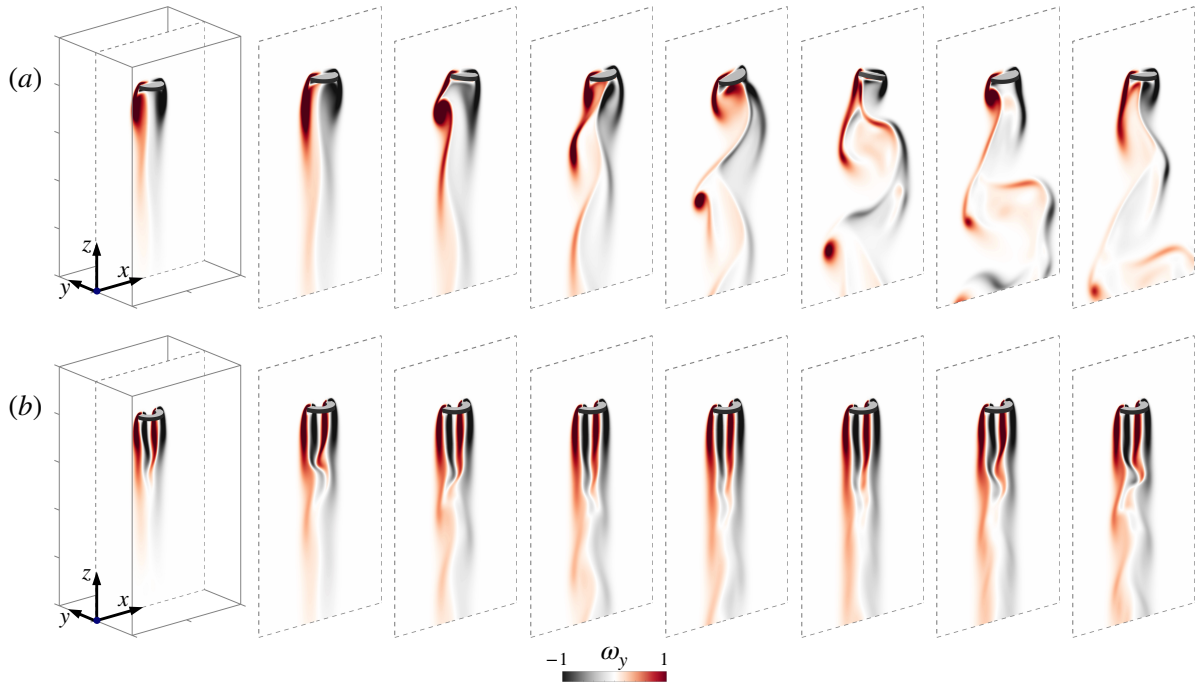


Figure 4.8: Spatio-temporal evolution of the vorticity profiles ω_y in the x - z plane with $Ar = 90$, $\chi = 7$ for a solid disc in panel (a) and a perforated ($d/D_D = 0.5$) disc in panel (b). The time history spans $tU/R_{eq} = 30$ to $tU/R_{eq} = 100$, with snapshots taken at intervals of $\Delta t = 10$. The results are shown on a slice in the y -normal direction, with a height of $9D_D$, extending from $1.8D_D$ above the disc to $7.2D_D$ below the disc.

terminal velocity, the vertical velocity V_z becomes essentially steady, with no discernible oscillations. Previous experimental studies [22, 152] have shown that introducing a central perforation can stabilise the motion of a disc at high Reynolds numbers. In particular, as d/D_D increases, a transition from a tumbling regime to a chaotic regime has been reported. Related regime changes have also been observed for discs with alternative perforation patterns [156] and for perforated plates [160].

Vincent et al. [22] reported that the stabilising influence of a central perforation becomes apparent once the hole reaches a critical size, with the transition occurring at approximately $d/D_D \simeq 0.3 \pm 0.1$. They further found that this regime change shifts to smaller values of d/D_D as the moment of inertia I^* decreases when fixing Re . Relative to the regime map for solid discs compiled by Field et al. [23], increasing d/D_D may therefore be interpreted as effectively lowering I^* at fixed Re [22]. An additional simulation is shown in Fig. 4.7 for $Ar = 49$ and $\chi = 7$ in a homogeneous fluid, where the area ratio is varied through d/D_D . The figure reports the time evolution of the lateral velocity component, V_x and the angular velocity $\dot{\theta}R_{eq}/U$. When the perforation is smaller ($d/D_D = 0.25$), fluttering persists with pronounced lateral oscillations, whereas for $d/D_D = 0.5$ the amplitude

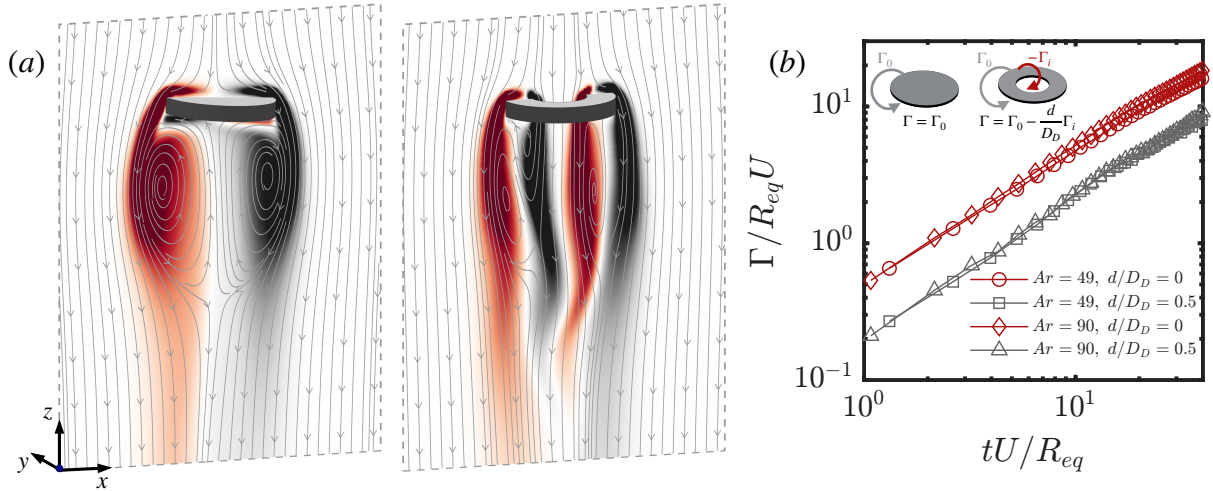


Figure 4.9: Panel (a) shows a close up comparison of the vorticity profile and the body frame streamlines with $Ar = 90$, $\chi = 7$ for a solid and perforated disc ($d/D_D = 0.5$) at $tU/R_{eq} = 30$. The colour map is the same as Fig. 4.8. The time history of the circulation Γ is presented in panel (b), where the inset illustrates the contributions to Γ for either case.

of V_x is strongly reduced, in agreement with the experimental observations of Vincent et al. [22] at high Re . We find that the phase angle, which quantifies the lag between the disc orientation and its direction of motion, is $\Delta\phi \approx 70^\circ$. This is consistent with previous measurements showing a strong dependence on aspect ratio; in particular, $\Delta\phi \gtrsim 90^\circ$ for sufficiently thin discs with $\chi \gtrsim 8$ ($\chi = 7$ in this work) [18, 154, 161].

When considering the flow field, Moffatt [162] posed the question of how the existence of holes may modify the wake dynamics of a disc, and, in turn, the instabilities associated with it. Recently, Zhang et al. [152] reported substantial differences in the wake of settling discs with multiple perforations, attributed to vortical structures shed from the holes. Here, Fig. 4.8 presents the temporal evolution of the flow field when $Ar = 90$, $\chi = 7$ in a homogeneous fluid. The development of the wake behind the disc is presented in the x - z plane from $tU/R_{eq} = 30$ up to $tU/R_{eq} = 100$ for a solid disc in panel (a) and a perforated disc with $d/D_D = 0.5$ in panel (b). A drastic difference between the wake structures is apparent in the vorticity field (ω_y). In panel (a), shear layers of opposite sign form behind the disc, and as the disc transitions to the fluttering regime after the initial transient, the wake becomes asymmetric and vortices are periodically shed downstream, with a shedding frequency comparable to that of the disc oscillation [154, 163]. In contrast, panel (b) shows that vorticity is generated not only at the outer rim of the disc (as in the impervious case) but also at the rim of the central hole. This produces an additional, oppositely signed toroidal vortex in the near wake, along with the primary vortex ring

attached to the outer edge. Vincent et al. [22] found in their high- Re experiments that the secondary counter-rotating vortex ring generated at the rim of the central hole plays a key role in the observed stabilisation, promoting the transition from a tumbling regime to a chaotic regime.

The role of the secondary vortex ring in the stabilisation process has been quantified through the circulation (here denoted as Γ) in Fig. 4.9, similarly to [22]. In panel (a) of Fig. 4.9, a close-up of the ω_y field in the x - z plane is shown for $tU/R_{eq} = 30$. Streamlines in the body reference frame are also included: they highlight the primary vortex ring attached to the outer rim in the solid disc case and, for the perforated disc, the presence of both this primary vortex ring and a secondary vortex ring associated with the inner rim. Here, Γ is evaluated during the initial stage of the simulation, from $tU/R_{eq} = 0$ to $tU/R_{eq} = 30$, as shown in panel (b) of Fig. 4.9. For solid discs, the contribution to Γ is solely derived from the primary vortex ring; we denote this contribution by Γ_0 , as indicated in the schematic in panel (b). For the perforated disc, both the primary and secondary vortex rings contribute to the effective circulation. Here, Γ_i denotes the circulation associated with the secondary vortex ring. The effective circulation is computed as [22]:

$$\Gamma = \Gamma_0 - \frac{d}{D_D} \Gamma_i. \quad (4.26)$$

The circulation is evaluated on a central x - z slice by integrating the y -component of vorticity over the fluid region. The slice is divided into left and right halves relative to the domain centreline, and positive and negative vorticity regions are treated separately. Weak background vorticity is excluded by retaining only connected regions whose vorticity exceeds a small fraction of the local peak magnitude on each side. For the impervious disc, the reported circulation is obtained by averaging the absolute contributions from the dominant vortex regions. In panel (b), the circulation for the solid discs collapses onto a single curve for both $Ar = 49$ and $Ar = 90$, while the perforated discs exhibit a lower circulation. When increasing d/D_D , the strength of the secondary vortex ring becomes comparable to that of the primary vortex ring, effectively reducing the flow induced torque experienced by the body causing the observed stabilisation.

4.4.2 Rising disc dynamics in a density-stratified ambient

Introducing background stratification adds additional complexities that are absent in a homogeneous environment. In a homogeneous fluid, a rising disc often approaches a terminal rise velocity and statistically steady behaviour after an initial transient. On the

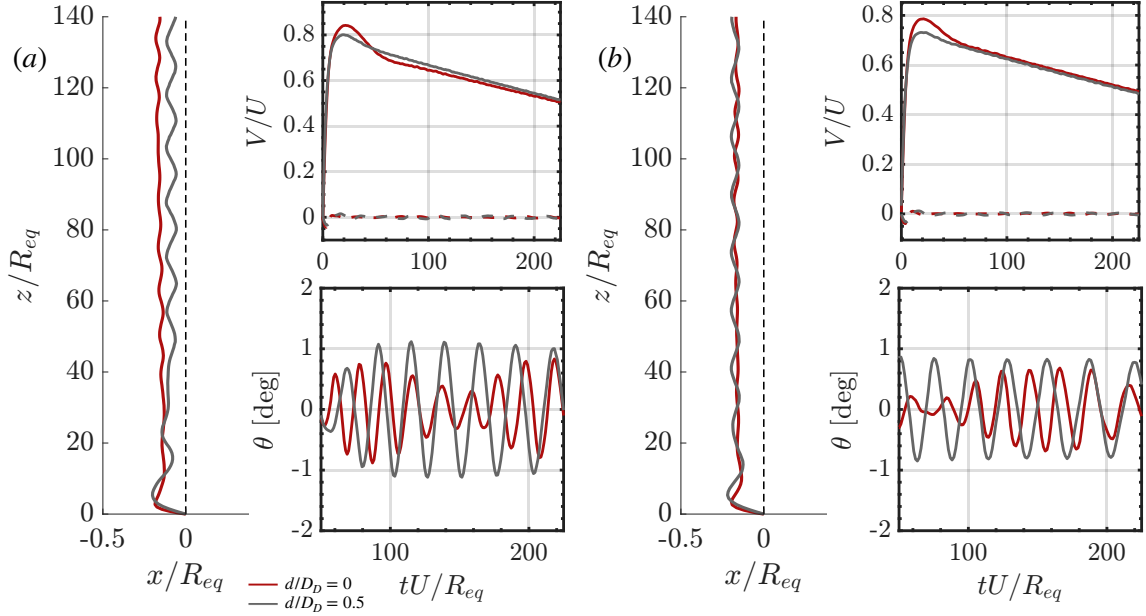


Figure 4.10: Disc trajectory in the x - z plane, time histories of the vertical (V_z , solid) and lateral (V_x , dashed) velocities, and the inclination angle θ for $Ar = 90$, $\chi = 7$, $Fr = 17$, $Sc = 0.7$, and $Ar = 49$, $\chi = 7$, $Fr = 17$, $Sc = 0.7$ shown in (a) and (b), respectively. Here, $I^* = 0.0072$ for solid discs, and $I^* = 0.0067$ for perforated discs.

other hand, dynamics remain height-dependent in a density-stratified fluid because the buoyancy force varies with the local fluid density $\rho_f(z)$. As a result, the disc may exhibit quasi-steady behavior over limited vertical intervals [37], but its rise velocity can continue to evolve as it ascends.

Stratification influences not only the vertical velocity but also the lateral drift and the inclination angle. Fig. 4.10 shows the side view (x - z plane), the vertical and lateral velocity components (V_z and V_x), and the inclination angle (θ) for four representative simulations when $Fr = 17$, $Sc = 0.7$, $\chi = 7$. Panel (a) corresponds to $Ar = 90$, and panel (b) corresponds to $Ar = 49$. Two main observations are made when comparing the disc dynamics in a density-stratified ambient and a homogeneous fluid. All four representative simulations show that as the disc rises, it attains a maximum rise velocity after the initial transient, followed by a monotonic decrease in the rising velocity. This behaviour has been observed previously for settling spheres [30], spheroids [35, 164], and impervious discs [37] in a linearly stratified fluid. Moreover, the oscillation amplitudes of the inclination angle ($\simeq \pm 1^\circ$) and the lateral displacement are suppressed relative to the homogeneous fluid cases for impervious discs. When perforated discs are considered, the peak velocity attained by the disc is slightly lower than that of a solid disc. This is attributed to the reduced perturbation of local ambient stratification due to the presence

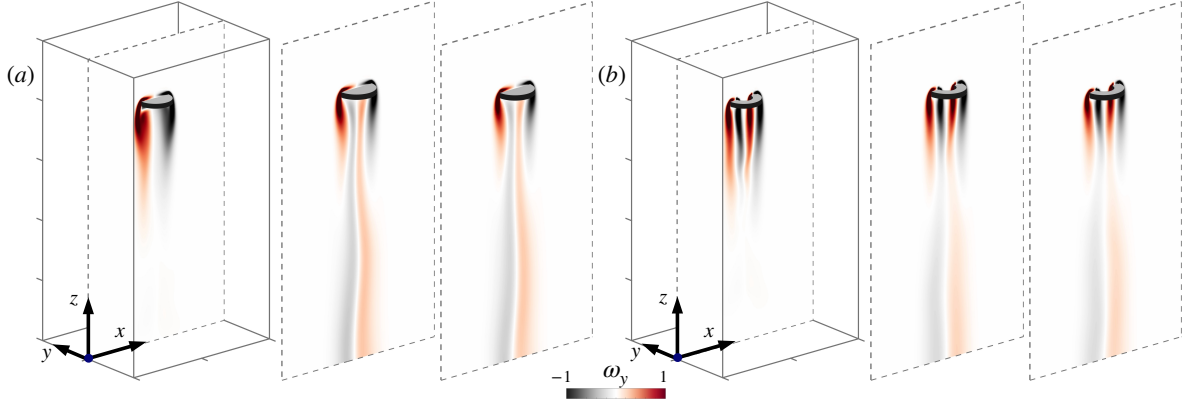


Figure 4.11: Spatio-temporal evolution of the vorticity profiles ω_y in the x - z plane with $Ar = 90$, $\chi = 7$, $Fr = 17$, $Sc = 0.7$ for a solid disc in panel (a) and a perforated ($d/D_D = 0.5$) disc in panel (b). The time history spans $tU/R_{eq} = 30$ to $tU/R_{eq} = 150$, with snapshots taken at intervals of $\Delta t = 60$. The results are shown on a slice in the y -normal direction, with a height of $9D_D$, extending from $1.8D_D$ above the disc to $7.2D_D$ below the disc.

of the hole, and the effect of which on the wake is presented in Figs. 4.11 and 4.12 for $Ar = 90$. In representative simulations, the oscillations of the inclination angle may also be influenced by the background stratification. However, the present parameter regime (moderate Fr) does not allow a clear separation between the intrinsic body oscillation of the disc and the stratification effects associated with the buoyancy frequency N [37].

By taking the curl of the momentum equation, the vorticity equation can be derived for density-stratified fluids under the Boussinesq approximation [12]:

$$\frac{D\boldsymbol{\omega}}{Dt} = (\boldsymbol{\omega} \cdot \nabla)\mathbf{u} + \nu \nabla^2 \boldsymbol{\omega} - \frac{g}{\rho_{f,0}} \nabla \rho_f \times \mathbf{e}_z, \quad (4.27)$$

where ν is the kinematic viscosity. In a density-stratified fluid, the last term on the right-hand side of Eq. (4.27) represents baroclinic vorticity generation arising from the local misalignment between the density gradient and the vertical direction. Note that, under the Boussinesq approximation, the baroclinic source term includes the hydrostatic contribution alone, compared to the usual term proportional to $\nabla \rho_f \times \nabla p$. In the present context, this term becomes significant when the rising disc distorts the ambient density field and the associated isopycnals.

Fig. 4.11 presents the temporal evolution of the disc rise at three different time steps for an impervious disc in panel (a) and a perforated disc in panel (b) ($Ar = 90$, $\chi = 7$, $Fr = 17$, $Sc = 0.7$). As the solid disc rises from rest, a primary vortex ring forms near the disc surface. The disc distorts the ambient density field, which promotes baroclinic

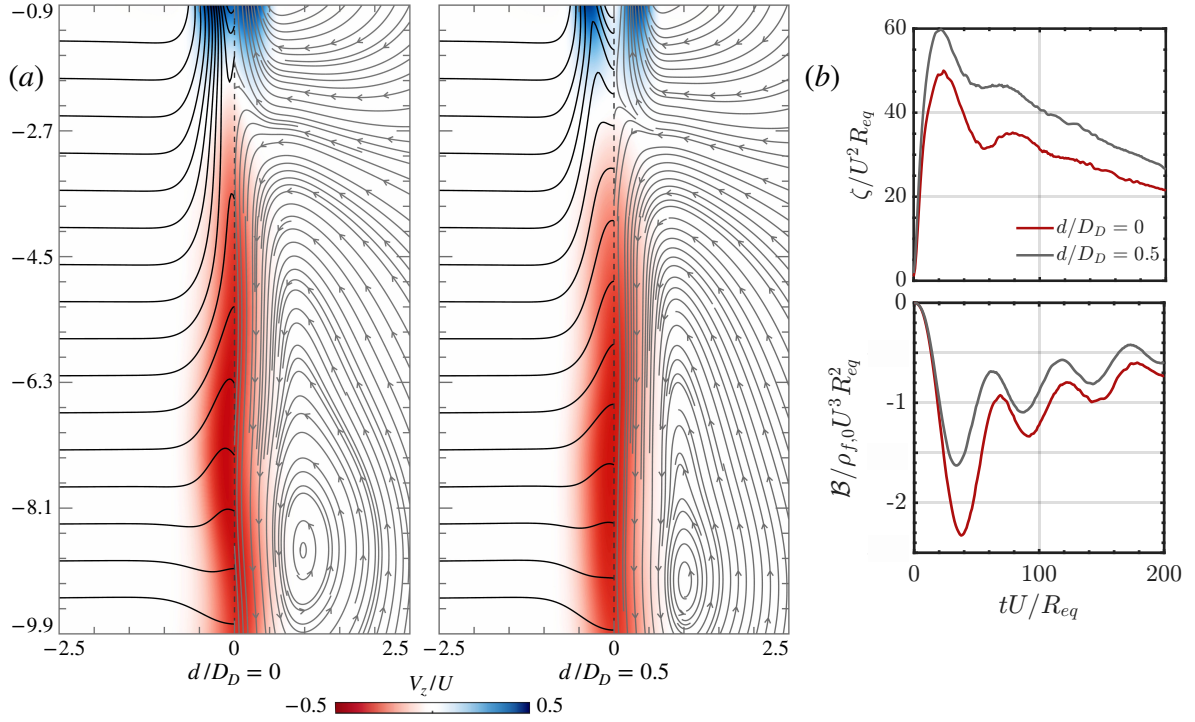


Figure 4.12: Panel (a) shows side views in the x - z plane of the wakes for a solid disc and a perforated disc with $d/D_D = 0.5$ in the stratified cases at $Ar = 90$, $\chi = 7$, $Fr = 17$, and $Sc = 0.7$ at $tU/R_{eq} = 150$. The axes are normalised by D_D and are with respect to the centre of mass of the disc. The left side presents the distorted isopycnals, and the right side shows the laboratory frame streamlines. Panel (b) shows the temporal evolution of the enstrophy ζ , and the buoyancy flux $\mathcal{B}$.

vorticity generation, leading to the formation of a buoyancy induced secondary toroidal vortex of opposite sign in the downstream wake [30, 35, 59, 164]. When the perforated disc rises, it initially forms a pair of counter-rotating vortices near the disc outer and inner edges. After some time, a toroidal vortex of opposite sign to the primary vortex ring develops downstream, in a manner similar to the solid disc case.

To further characterise the wake dynamics in a density-stratified fluid, the velocity field downstream of the disc is presented in Fig. 4.12 at $tU/R_{eq} = 150$ in the x - z plane. Panel (a) shows the wake of the solid and perforated disc, with the associated isopycnals on the left and the laboratory-frame streamlines on the right. The axes are normalised by D_D and are with respect to the centre of mass of the disc. In a density-stratified fluid, Torres et al. [32] found complete collapse of the rear vortex when increasing the role of stratification (decreasing Fr). However, that does not mean the flow is irrotational, as can be seen from the laboratory frame streamlines, where a region of large vorticity exists in the wake of the disc. A region of positive velocity is observed near the disc surface in both the impervious and perforated cases, associated with the disc rise. The isopyc-

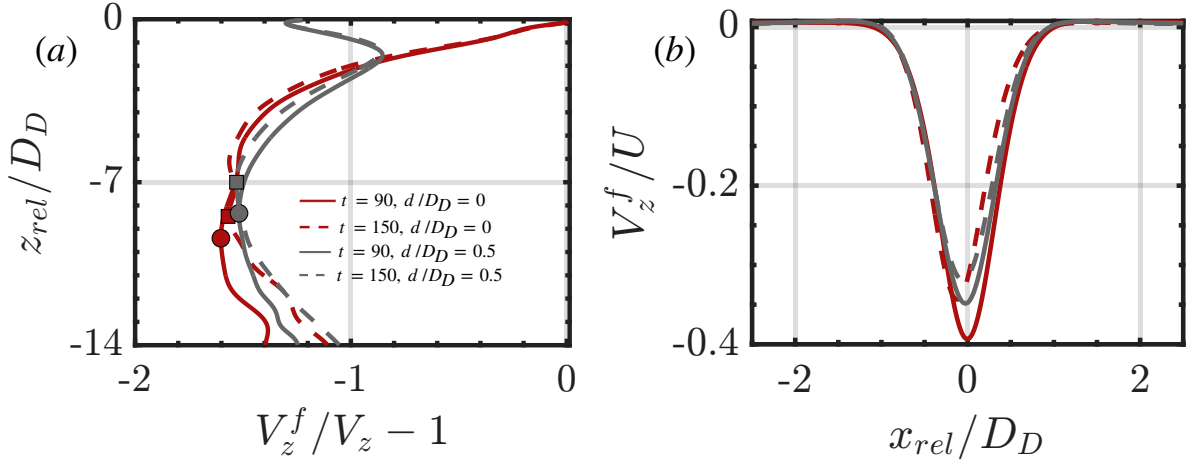


Figure 4.13: Panel (a) shows the centreline profile of the relative wake vertical velocity $V_z^f/V_z - 1$ as a function of z_{rel} , the vertical coordinate measured relative to the disc centre at its instantaneous height, for $Ar = 90$, $\chi = 7$, $Fr = 17$, and $Sc = 0.7$ at $tU/R_{eq} = 90$ and $tU/R_{eq} = 150$. Markers indicate the relative vertical position z_{rel} at which V_z^f attains its minimum. Circles correspond to $tU/R_{eq} = 90$, and squares correspond to $tU/R_{eq} = 150$. Panel (b) shows the lateral profile of V_z^f along the x direction evaluated at these marker locations.

nals are distorted in the near wake, and as they return towards their neutrally buoyant position, a region of negative velocity develops downstream of the disc. Furthermore, comparing the distorted isopycnals in the solid and perforated cases reveals that, immediately downstream of the disc, there is a region of reduced isopycnal displacement for the perforated disc case.

Fig. 4.12(b) shows the time histories of the enstrophy, ζ , and the volume-integrated buoyancy flux, $\mathcal{B}$, which are respectively given by

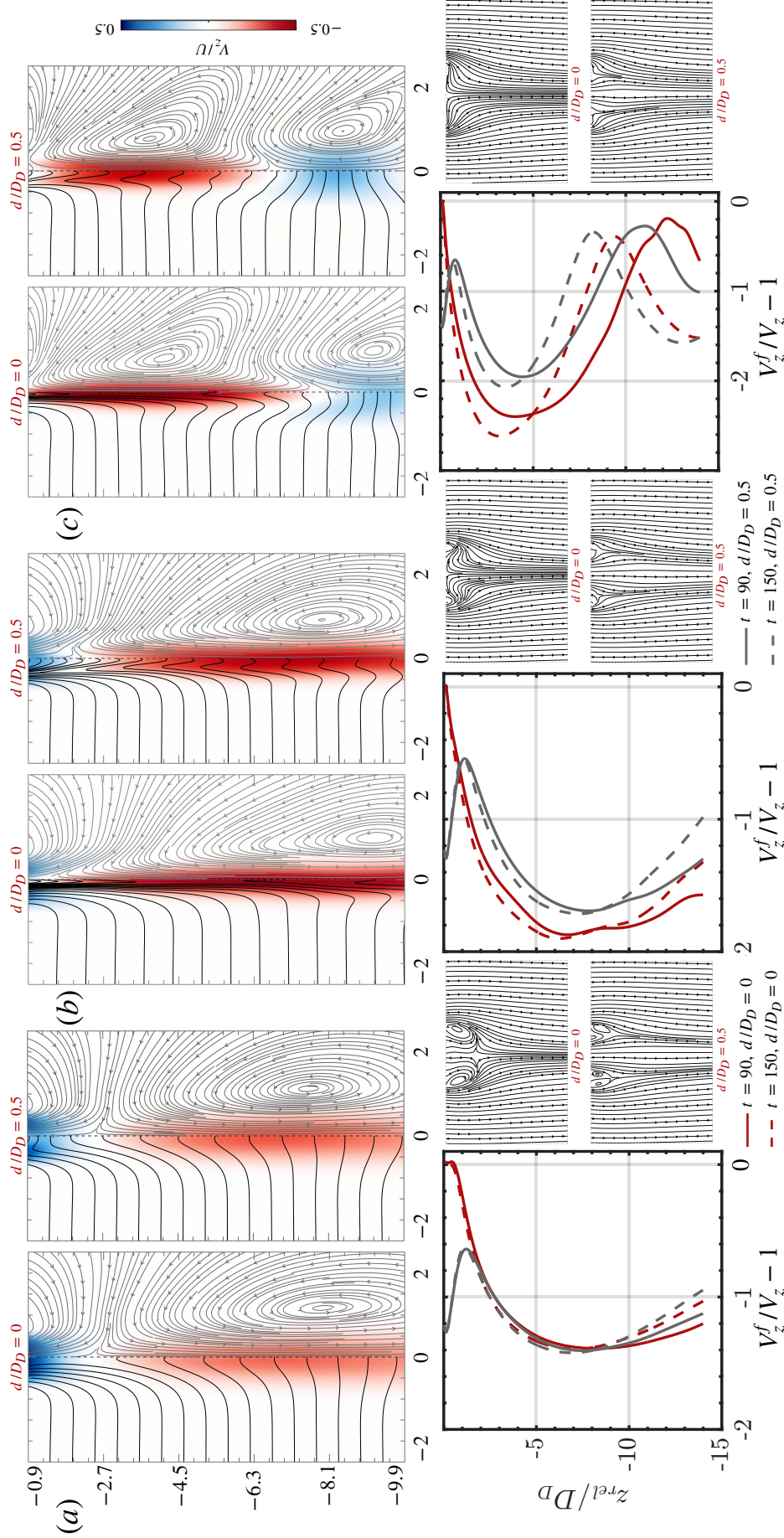
$$\zeta = \frac{1}{2} \int_V \|\boldsymbol{\omega}\|^2 dV, \quad (4.28)$$

$$\mathcal{B} = -g \int_V V_z^f \rho'_f dV, \quad (4.29)$$

where $\|\boldsymbol{\omega}\|^2 = \boldsymbol{\omega} \cdot \boldsymbol{\omega}$ and ρ'_f is the density anomaly. In a density-stratified fluid, the buoyancy flux quantifies the reversible exchange between kinetic and potential energy [165] and is linked to baroclinic vorticity production. Comparing the buoyancy flux between the solid and perforated discs reveals that $|\mathcal{B}|$ is larger for the solid disc. This indicates a stronger generation of baroclinic vorticity in the solid disc wake, consistent with the larger perturbation of the ambient density field (more exchange from kinetic to potential energy). However, enstrophy, which measures the intensity of rotational flow, is larger at all times when $d/D_D = 0.5$, attributed to the vorticity produced near the disc hole.

In panel (a) of Fig. 4.13, the relative velocity of the fluid ($V_z^f/V_z - 1$) along the centreline of the wake is presented at two different time steps when $Ar = 90$, $Fr = 17$, $Sc = 0.7$, where the markers represent the axial positions of the maximum $|V_z^f|$. In panel (b), a transverse plot along the region indicated by the markers of panel (a) is presented. Panel (b) shows that the maximum fluid velocity magnitude in the caudal (jet) region of the disc wake is smaller when a perforation is introduced into the disc, consistent with the observations made in Fig. 4.12. A standing eddy, which corresponds to a relative velocity ($V_z^f/V_z - 1$) greater than zero near the disc surface (close to $z_{rel} = 0$) for the impervious disc, is not found for $Ar = 90$ similar to the findings of Zhang et al. [14] for settling spheres when $Re = 100$. When $d/D_D = 0.5$, a region of downward axial velocity is observed in the near wake, immediately adjacent to the disc. This behavior is a direct consequence of the disc permeability. As the disc rises, a pressure difference between the upstream and downstream faces drives a finite throughput across the disc. The resulting flow through the perforation introduces downward momentum into the wake in the immediate vicinity of the disc, yielding negative V_z^f along the wake centreline. In the disc frame, this manifests itself as a relative velocity ($V_z^f/V_z - 1$) < -1 near $z_{rel} \approx 0$ compared to the impervious disc. From panel (a), it can be seen that the stratification induced localised jet downstream of the disc is slightly shorter when introducing the perforation. A similar behaviour is found in Fig. 4.14 when comparing the flow field when $Ar = 49$ at $tU/R_{eq} = 150$, where panel (a) corresponds to ($Sc = 0.7$, $Fr = 17$), panel (b) to ($Sc = 7$, $Fr = 17$) and panel (c) to ($Sc = 7$, $Fr = 11.4$).

When decreasing Ar while keeping (Sc , Fr) fixed, the jet region of the wake follows the same trend as in Fig. 4.13. However, closer to the disc surface, the impervious disc case shows a slightly positive $V_z^f/V_z - 1$, indicating that the standing eddy persists under these conditions and has not completely collapsed. This can be visualised through the body frame streamline adjacent to the disc surface. Decreasing the diffusivity of the stratifying agent (increasing Sc) leads to a more pronounced distortion of the ambient density field, visible as stronger isopycnal deformation. The resulting increase in the axial density gradient intensifies the generation of baroclinic vorticity, which, in turn, strengthens the jet by increasing its peak velocity magnitude.



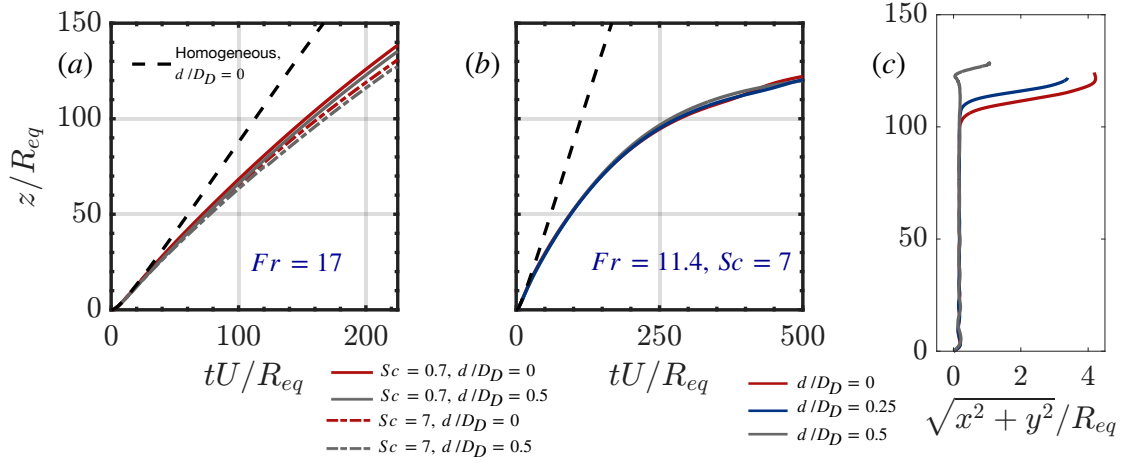


Figure 4.15: Time histories of the disc's instantaneous vertical position are shown for (a) $Ar = 49$ at $Fr = 17$ with $Sc = 0.7$ and $Sc = 7$, for both $d/D_D = 0$ and $d/D_D = 0.5$, and (b) $Ar = 49, Sc = 7, Fr = 11.4$ for $d/D_D = 0, 0.25$, and 0.5 . Panel (c) shows the corresponding rise trajectories for the cases in panel (b).

The collapse of the standing eddy is stronger when increasing Sc , and the discrepancy in the jet strength between the impervious and perforated discs becomes more pronounced, evidenced by a larger separation in the profiles of $V_z^f/V_z - 1$. When decreasing Fr , panel (c) shows the complete collapse of the standing eddy, as seen by Torres et al. [32] when decreasing Fr . Decreasing Fr leads to an increase in the potential energy attained by the fluid parts, so that the exchange between the fluid potential and the kinetic energy is stronger. As a result, the strength of the jet intensifies as Fr decreases, as seen both in the velocity field and in the centreline profile of the relative velocity. The disparity between impervious and perforated cases also grows, affecting both the jet length and its associated velocity profile.

The effect of varying Sc is considerable when visualising the wakes in panels (a) and (b) of Fig. 4.14, however the influence of stratification on the disc rising dynamics is rooted in the fluid buoyancy force, which if left constant, leads to a similar behaviour as observed in panel (a) of Fig. 4.15. This was also found for settling spheroids in density-stratified fluids [35]. However, for settling spheres or rising droplets, the vertical velocity oscillation with an oscillation frequency related to N was found in strongly stratified fluids. The observed oscillations have a nontrivial effect on Sc , as they are largely induced by the displaced ambient density field.

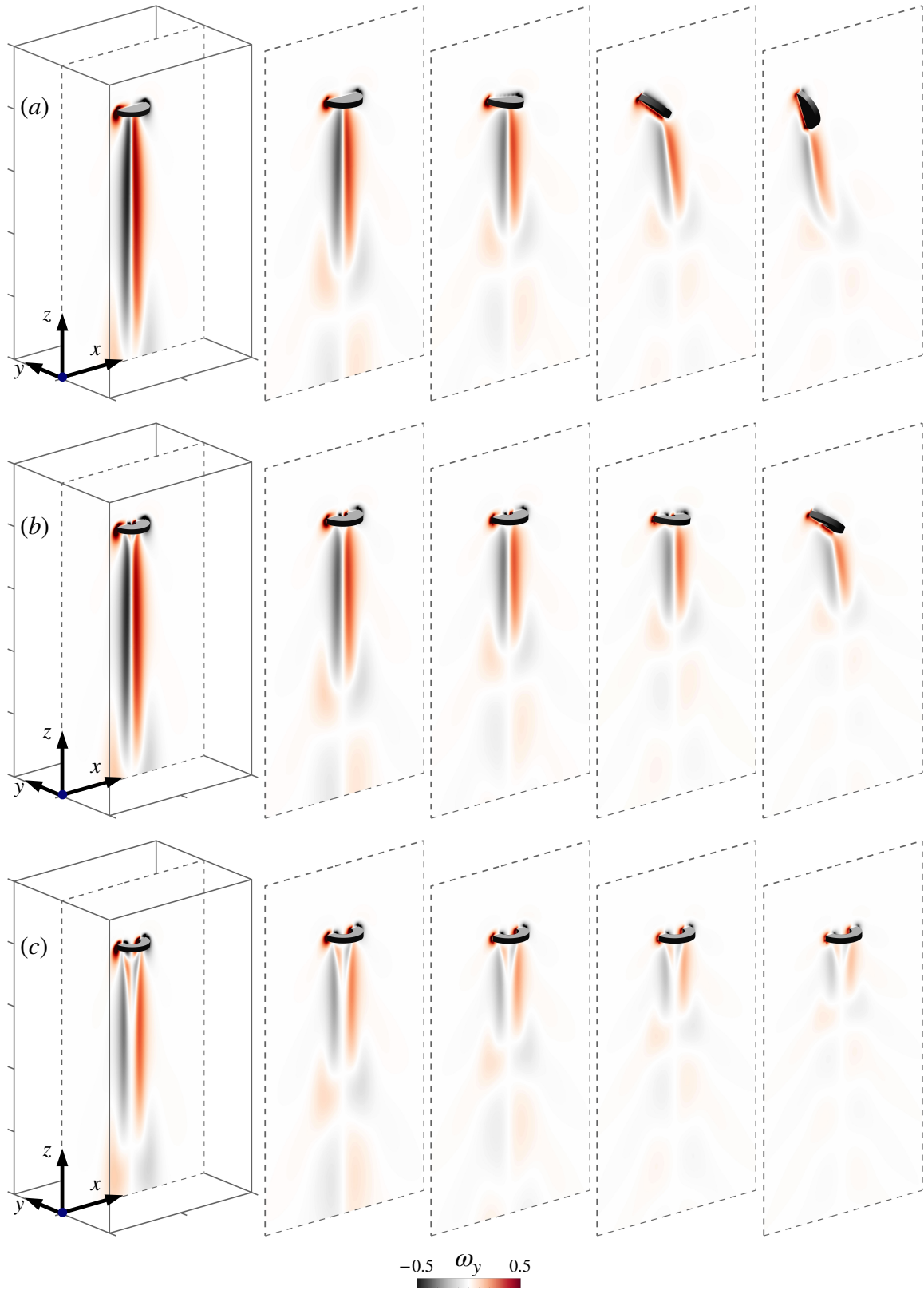


Figure 4.16: Spatiotemporal evolution of the vorticity field ω_y for $Ar = 49$, $Sc = 7$, $Fr = 11.4$ when (a) $d/D_D = 0$, (b) $d/D_D = 0.25$ and (c) $d/D_D = 0.5$. From left to right, $tU/R_{eq} = [200, 300, 350, 400, 450]$.

When increasing the stratification strength, the disc rises with heavier fluid surrounding the disc surface into a position of lighter fluid. In turn, the increased deceleration of the disc associated with the increased difference in fluid buoyancy force can be seen in panel (b) of Fig. 4.15, which presents the instantaneous vertical position of the disc when varying d/D_D . Furthermore, discs and spheroids have been shown to reorient from the stable broadside-on configuration observed in a homogeneous fluid to an edgewise configuration when the stratification is sufficiently strong. Here, an edgewise orientation denotes a configuration in which the disc presents a minimal projected area to the direction of motion, denoted by $\theta = 90^\circ$. The change in stability that governs the reorientation of discs and spheroids in linearly stratified fluids has previously been reported to occur after the magnitude of the particle velocity drops below a certain threshold. The reorientation of the particle is associated with the dominance of buoyancy induced torque over the hydrodynamic torque.

More et al. [35] has found that the threshold velocity required for spheroids to reorient depends on the Galilei and Richardson numbers (Ar and Fr in this work). Moreover, the process of reorientation is accompanied by lateral (in-plane) drift, prior to the particle reaching its neutrally buoyant position. This is observed when considering panel (c) of Fig. 4.15 after the initial broadside-on rising phase. Panel (c) further shows that the onset of lateral drift varies with increasing d/D_D , so that the disc reaches a higher vertical position, where the ambient fluid density is lower, with a broadside-on orientation.

Fig. 4.16 presents the time histories of the vorticity field ω_y for $Ar = 49$, $Sc = 7$, $Fr = 11.4$ when (a) $d/D_D = 0$, (b) $d/D_D = 0.25$ and (c) $d/D_D = 0.5$. As the particle continues to decelerate after attaining its peak velocity, the vorticity magnitude in the caudal region associated with baroclinic torque decreases over time. Close to the disc centreline, a thin ‘plume’, which designates the region where $\omega_y = 0$ and separates the regions of positive and negative vorticity, can be seen for all three cases. Comparing panels (b) and (c) to panel (a), it can be seen that the transverse thickness of this plume increases with increasing d/D_D . More et al. [35] associated the reorientation observed in settling spheroids with the departure of the plume from the spheroid’s centreline. A similar observation can be seen here at later times in panels (a) and (b), where as the disc begins to reorient, a shift in the position of the plume from close to the centreline of the disc towards the edge of the disc induces an additional torque on the disc, amplifying its reorientation [37]. Comparing the later time dynamics ($tU/R_{eq} = 450$), it can be seen that when $d/D_D = 0$ and $d/D_D = 0.25$, the discs have at least started to reorient. However, this reorientation was not observed until later when $d/D_D = 0.5$ ($tU/R_{eq} = 579$), as presented in panel (a) of Fig. 4.17. The time at the onset of reorientation (here taken at

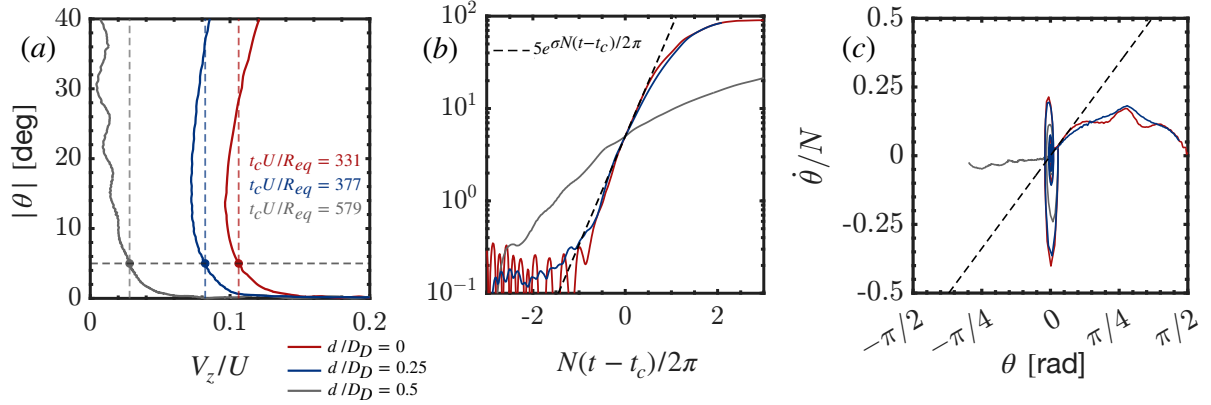


Figure 4.17: Panels (a) and (b) present the time history of $|\theta|$ with respect to V_z/U and $N(t - t_c)/2\pi$, respectively. Here t_c is the time where $\theta = 5^\circ$ during the reorientation process. The dashed line in panel (b) corresponds to $5e^{\sigma N(t-t_c)/2\pi}$, where $\sigma = 2.7$ as per the experiments of Mercier et al. [37]. In panel (c), the phase diagram of the angular velocity and the orientation angle is presented, where the dashed line has a slope of $\sigma/2\pi$. The results here correspond to $Ar = 49$, $Sc = 7$, $Fr = 11.4$ and varying d/D_D .

$\theta = 5^\circ$ after the broadside rising phase) in Fig. 4.17 is denoted by t_c . A clear trend can be seen, where t_c increases with increasing disc permeability, indicating that the broadside regime becomes more stable as the disc tends towards the shape of a thin ring (increasing d/D_D). Panel (a) shows that as t_c increases with increasing d/D_D , the threshold velocity required for the reorientation process decreases. Although outside the scope of the current work, it would be interesting to consider the role of different styles of perforations on the onset or suppression of the reorientation process in a density-stratified ambient.

In panels (b) and (c) of Fig. 4.17, the temporal evolution of the magnitude of θ and the phase diagram of the angular velocity with respect to the orientation angle are presented. From simulations and experiments of Mercier et al. [37] for solid discs settling in a linearly stratified environment, it was shown that as the disc settles, there is a convergence towards $(\theta, \dot{\theta}) = (0, 0)$ prior to the start of reorientation. A similar convergence can be seen here during the broadside-on rising phase, attributed to the suppression of flutter induced by ambient stratification [40].

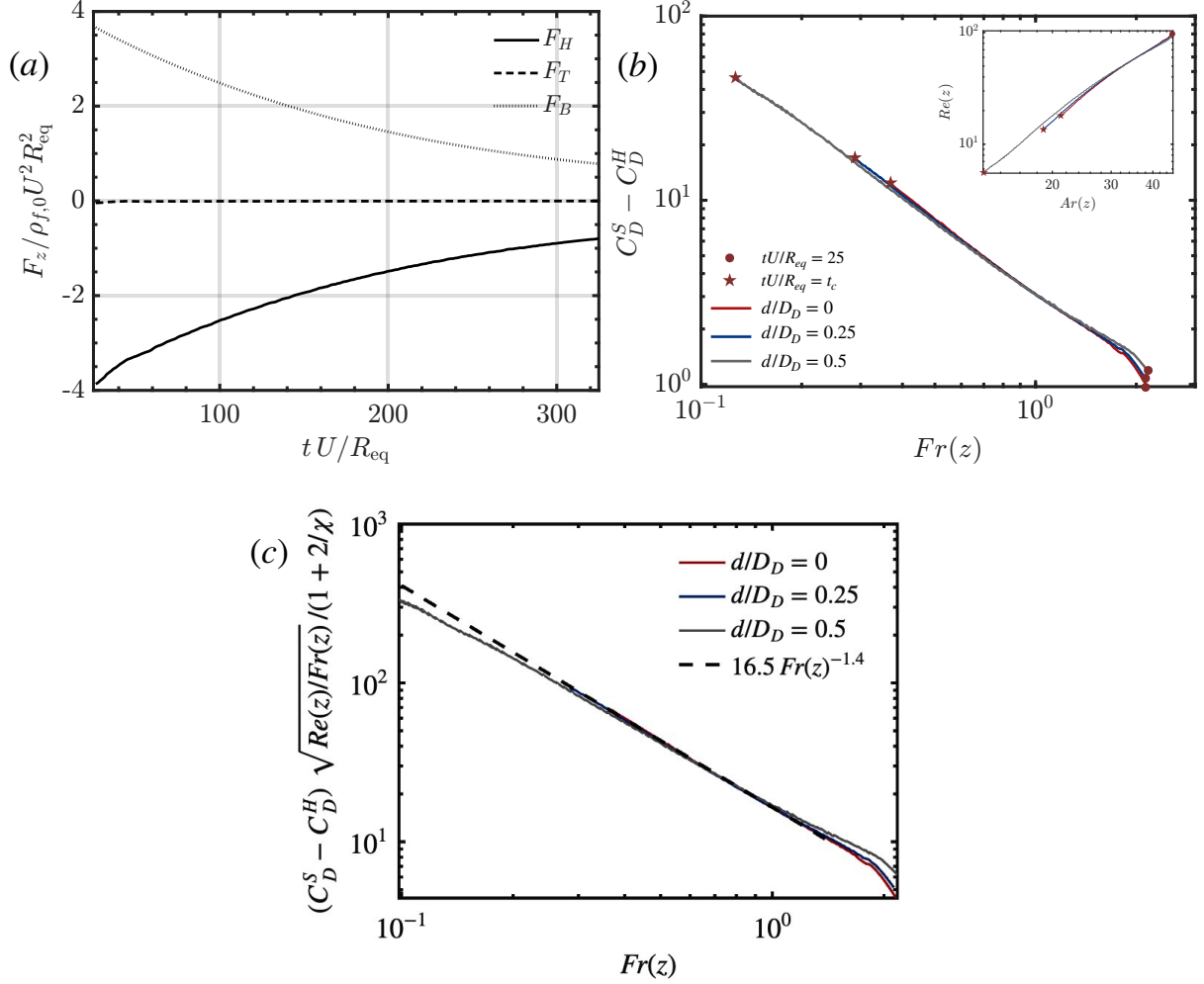


Figure 4.18: Panel (a) presents a force decomposition (z -direction) from $tU/R_{eq} = 25$ to $t = t_c$ when $Ar = 49$, $Sc = 7$, $Fr = 11.4$, and $d/D_D = 0$, illustrating quasi-steady behaviour. Panel (b) shows the evolution of $C_D^S - C_D^H$ as a function of the instantaneous Froude number $Fr(z)$. The inset in panel (b) presents the instantaneous Reynolds against Archimedes numbers. Under quasi-steady state, $C_D^S = \frac{32 Ar(z)^2}{3 Re(z)^2}$. The cases in panel (b) are for $Ar = 49$, $Sc = 7$, $Fr = 11.4$ and varying d/D_D . Panel (c) shows the stratification-induced drag enhancement, $(C_D^S - C_D^H) \sqrt{Re(z)/Fr(z)} / (1 + 2/\chi)$, as a function of the instantaneous Froude number $Fr(z)$. The dashed line denotes a power-law fit, $16.5 Fr(z)^{-1.4}$.

Furthermore, from the experimental results of Mercier et al. [37], the onset of impervious disc reorientation can be modelled with exponential growth $\theta(t) = 5e^{\sigma N(t-t_c)/2\pi}$, where σ is the growth rate. Their experiments have shown that $\sigma = 2.7$ best matches the initial reorientation process. The dashed lines in panels (b) and (c) correspond to this model, where $\sigma = 2.7$ was taken according to the experiments. From panel (b), it can be seen that for the impervious case, this growth rate is in excellent agreement with our numerical results for early times. However, when increasing d/D_D , the growth rate decreases slightly for $d/D_D = 0.25$ and substantially when $d/D_D = 0.5$. The decrease in growth rate is directly related to the vorticity profile observed in Fig. 4.16. As the disc begins to reorient due to the dominance of the buoyancy torque over its hydrodynamic counterpart [35], the misalignment between the centre of the plume and the centre of the impervious disc accelerates the reorientation process. As d/D_D increases, the plume becomes transversely broader and the offset between the disc centreline and the plume centre decreases, thus weakening the driving mechanism for accelerated reorientation.

Lastly, settling and rising bodies in density-stratified fluids experience enhanced drag due to stratification [14, 37, 54]. To quantify the enhanced drag in a density-stratified fluid, we assume that the rising discs are in a quasi-steady state, which is valid predominantly during the broadside-on rising phase of the disc after the discs have attained their peak velocity. In panel (a) of Fig. 4.18, we plot the temporal evolution of the buoyancy force $F_B = \int_V \rho_f g dV - \rho_p \mathcal{V}g$, the total force in the rising direction $F_T = \rho_p \mathcal{V} dV_z/dt$ and the hydrodynamic force in the rising direction $F_H = \int_S \boldsymbol{\tau} \cdot \mathbf{n} dS$, where $\boldsymbol{\tau}$ is the stress tensor and $\mathbf{n}$ is the outward facing normal. From panel (a), it can be seen that the hydrodynamic and buoyancy forces are the two dominant forces during the broadside-on rising phase since F_T is close to zero, which validates the quasi-steady state assumption. Hence, neglecting added-mass and history terms, a stratification induced drag coefficient (C_D^S) can be defined following Yick et al. [54]:

$$C_D^S = \frac{2|\hat{\rho}|gh}{V_z^2}. \quad (4.30)$$

Furthermore, an instantaneous Archimedes, Reynolds, and Froude numbers may be defined as:

$$Ar(z) = \sqrt{\frac{3}{16}} \frac{\sqrt{gh|\hat{\rho}|(D_D^2 - d^2)}}{\nu}, \quad (4.31)$$

$$Re(z) = \frac{|V_z|\sqrt{D_D^2 - d^2}}{\nu}, \quad (4.32)$$

$$Fr(z) = \frac{|V_z|}{N\sqrt{D_D^2 - d^2}}. \quad (4.33)$$

A drag coefficient C_D^H defined previously in Eq. (4.23) can be utilised as it models the drag coefficient of a disc in a homogeneous fluid ($Fr \rightarrow \infty$). Panel (b) of Fig. 4.18 presents $C_D^S - C_D^H$ when varying d/D_D as a function of $Fr(z)$ from $tU/R_{eq} = 25$ up to t_c . As $tU/R_{eq} = 25$ corresponds to a time close to that at which the discs attain their maximum velocity, it corresponds to the point of highest $Fr(z)$ and lowest $C_D^S - C_D^H$. As buoyancy effects become stronger, the stratification-induced drag coefficient increases as the particle speed decreases, which in turn reduces $Fr(z)$. Panel (b) shows that the stratification induced enhancement to the drag coefficient can be significantly larger than its homogeneous counterpart [35, 37, 164], with no discernible difference when increasing d/D_D .

To further assess whether the present stratification-induced drag follows the scaling proposed by Mercier et al. [37], the same data are replotted using the normalised ordinate in panel (c),

$$Y = (C_D^S - C_D^H) \frac{\sqrt{Re(z)/Fr(z)}}{1 + 2/\chi}. \quad (4.34)$$

This normalisation follows from the argument of Mercier et al. [37], in which the additional drag is associated with a thin shell of displaced light fluid entrained with the disc. For a disc, the entrained volume introduces the geometrical factor $(1 + 2/\chi)$, while the shell thickness scales as $\delta/D_D \sim \sqrt{Fr/Re}$. Under this rearrangement, their model reduces to

$$Y = aFr(z)^q, \quad (4.35)$$

with $a = 14 \pm 2$ and $q = -1.7 \pm 0.1$ for their fitted parameter range. The present solid and annular disc data collapse reasonably well under the same normalisation, indicating that the dominant dependence of the stratification-induced drag remains captured by the scaling of Mercier et al. [37] during the broadside quasi-steady phase. A power-law fit to the present data gives $Y = 16.5Fr(z)^{-1.4}$, which is close in magnitude but slightly shallower than the fit of Mercier et al. [37]. The difference between the present fitted relation and that of Mercier et al. [37] may be attributed, at least in part, to the smaller Schmidt number considered here, as the reference correlation was obtained over higher- Sc conditions and a broader parameter range.

4.5 Concluding remarks

This chapter starts by considering benchmark tests for settling isolated spheres in both homogeneous and density-stratified fluids, where excellent agreement is found compared

to the results found in the literature. Furthermore, we consider the rise dynamics of solid and annular discs in homogeneous and linearly stratified fluids at moderate Reynolds numbers. First, for impervious discs in a homogeneous fluid, our numerical results are benchmarked against the experiments of Fernandes et al. [19], showing excellent agreement in the homogeneous drag coefficient, C_D^H . Introducing a central perforation leads, for $Ar = 49$ and $Ar = 90$, to a transition from a fluttering trajectory to rectilinear rise, consistent with the stabilising influence of holes reported by Vincent et al. [22] at high Re . The stabilising effect of the perforation was quantified through the circulation Γ , by isolating the contributions of the primary and secondary counter-rotating vortex rings. In addition, perforation yields a slight increase in C_D^H , consistent with the reduced projected area.

In the linearly stratified cases, we analyse the wake dynamics by examining vorticity fields and centreline velocity profiles. Consistent with previous studies in stratified ambient fluids, the rise generates an additional detached toroidal vortex in the wake, attributable to the production of baroclinic vorticity. Under sufficiently strong stratification (small Fr), discs and spheroids are known to undergo an orientational instability, transitioning from a broadside-on configuration to an edgewise orientation; this reorientation is also observed here. Increasing the size of the perforation, d/D_D , delays the onset of instability and reduces the critical (threshold) velocity at which reorientation begins. The growth rate of this instability was found to decrease with increasing d/D_D , attributed to the alignment between the centre of the disc and the stratification induced vortex plume.

The present results may be relevant to a range of oceanic settings in which stratification modifies both wake dynamics and body orientation. For example, the ability of stratification and perforations to suppress fluttering dynamics, while altering lateral dispersion, is directly relevant to the passive deployment of ocean-monitoring sensors and drifters for which platform orientation and trajectory stability are important [166]. The findings also have implications for the transport of microplastics and other porous or damaged fragments in the ocean: perforation/porosity provides a simple proxy for weathered particles, and our results suggest that such geometric features can modify wake strength and delay the onset of reorientation near pycnoclines, potentially affecting residence times and lateral dispersion in stratified layers.

Chapter 5

The role of particle interactions in a density-stratified fluid

Contents

5.1	Introduction	93
5.2	Benchmark tests	96
5.2.1	Boussinesq approximation: Validation	98
5.3	In-line spheroids in a density-stratified fluid	99
5.3.1	Settling behaviour	99
5.3.2	Flow field and particle dynamics	105
5.3.3	Role of Sc	114
5.3.4	Crossing the density transition	115
5.3.5	Role of Ar	119
5.4	Increasing N_p for spheres	120
5.5	Concluding remarks	130

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5.1 Introduction

Following the previous chapter, which examined the dynamics of isolated discs in stratified fluids, this chapter considers the settling of two spheroidal particles that are initially aligned one behind the other (in-line) in a linearly stratified fluid. It investigates how the stratification strength, the particle aspect ratio, and the initial separation distance influence the settling dynamics. We then extend the discussion by increasing the particle number, considering a sparse cluster of spheres, drawing comparisons to previous experiments in homogeneous fluids. The remainder of this chapter is organised as follows. It first presents the problem formulation and benchmark tests. It then discusses the numerical results. Finally, it closes with concluding remarks.

We scale space, velocity, time, and vorticity on D_{eq} , $U = \sqrt{D_{eq}|\rho_p/\rho_{f,0} - 1|g}$, $\sqrt{D_{eq}/g}$, and $\sqrt{g/D_{eq}}$, respectively, so that the non-dimensional parameters governing the problem are the Archimedes, Froude, and Schmidt numbers, respectively given by

$$Ar = \frac{D_{eq}U\rho_{f,0}}{\mu_f}, \quad Fr = \frac{U}{ND_{eq}}, \quad Sc = \frac{\mu_f}{\rho_{f,0}\kappa}; \quad (5.1)$$

here, $N = \sqrt{-g\gamma/\rho_{f,0}}$ is the Brunt-Väisälä frequency, and the limit $Fr \rightarrow \infty$ corresponds to the unstratified homogeneous fluid case. Furthermore, D_{eq} denotes the volume-equivalent diameter of a spherical particle. In Section 5.3 of this chapter, we set $\rho_p = 1141 \text{ kg/m}^3$ and $\rho_{f,0} = 1000 \text{ kg/m}^3$, and fix the fluid viscosity at $\mu_f = 0.001 \text{ kg m}^{-1} \text{ s}^{-1}$. We also set $Sc = 700$, which corresponds to a salinity-stratified fluid, and obtain solutions for $Ar = 4.65$ and $2 \leq Fr \leq 12$. MacIntyre et al. [15] observed that particles and marine snow in the ocean settle with Reynolds numbers ranging from 0.2 to 23 and Froude numbers between 5 and 70. Furthermore, we investigate the effects of varying the particle aspect ratio on the settling behaviour, considering a particle size and background fluid stratification strengths similar to those found in the ocean. Using the above scaling, the dimensionless version of the initial density profile reads:

$$\tilde{\rho}_f = 1 - \frac{|\rho_p/\rho_{f,0} - 1|}{Fr^2} \tilde{z}, \quad (5.2)$$

where the tildes, which designate dimensionless variables, are suppressed henceforth. The roles of Sc and Ar are considered in Sections 5.3.3 and 5.3.5, respectively. When considering a sparse cluster of spheres in Section 5.4, the simulation setups are discussed therein.

The particle shape is characterised by its aspect ratio, $\mathcal{AR}$, defined as $\mathcal{AR} = a/b$,

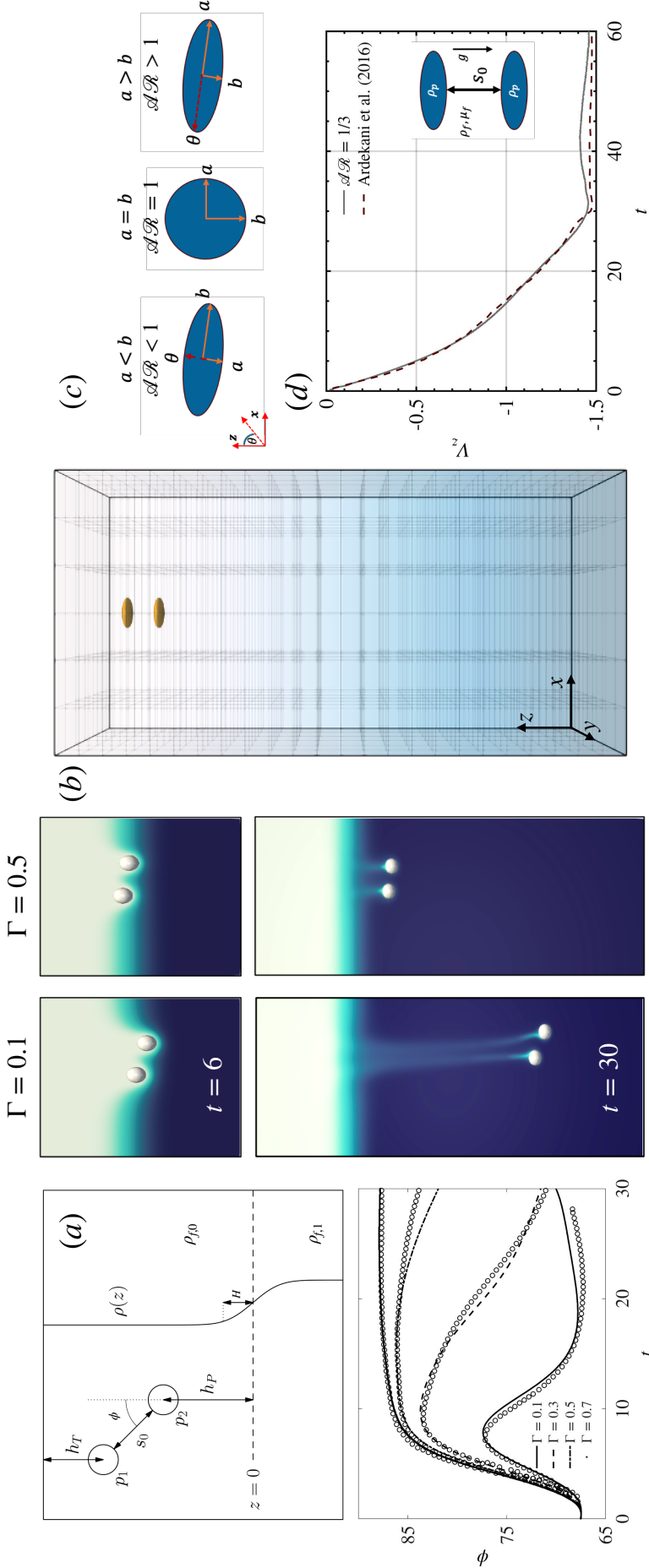


Figure 5.1: Panel (a) compares our numerical predictions with those of Deepwell et al. [16], for a spherical particle pair settling in a sharply stratified fluid. The simulation setup with the required definitions are provided as an illustration (adapted from Deepwell et al. [16]), and the numerical results for the angle ϕ between the two particles is presented when varying Γ (the markers correspond to the results of Deepwell et al. [16]). Qualitative results for two simulations ($\Gamma = 0.1$ and $\Gamma = 0.5$) at $t = 6$ and $t = 30$ are also presented. The particle Reynolds number (using the Stokes velocity scale) was set at $Re = 1/4$, Sc was fixed at 700, and the initial orientation angle ϕ was set at 67.5° . In panel (b), the simulation setup for oblate spheroids settling in-line is presented showcasing the subdomain decomposition and the background colour map illustrates the linear background density field. In panel (c), a schematic of the spheroidal axes are presented, where the polar radius of the spheroid is denoted as (a) , and the equatorial radius as (b) . The definitions of the aspect ratio ($\mathcal{AR} = a/b$) and the polar angle (θ) are also presented, where $\mathcal{AR} < 1$ is for an oblate spheroid, $\mathcal{AR} = 1$ is for a sphere, and $\mathcal{AR} > 1$ is for a prolate spheroid. In panel (d), a schematic of the initial separation distance between the leading and trailing particles (s_0) is presented, and a comparison of the average settling velocity V_z for a pair of oblate spheroidal particles with $\mathcal{AR} = 1/3$ with the numerical results of Ardekani et al. [41] is presented for $Ar = 80$.

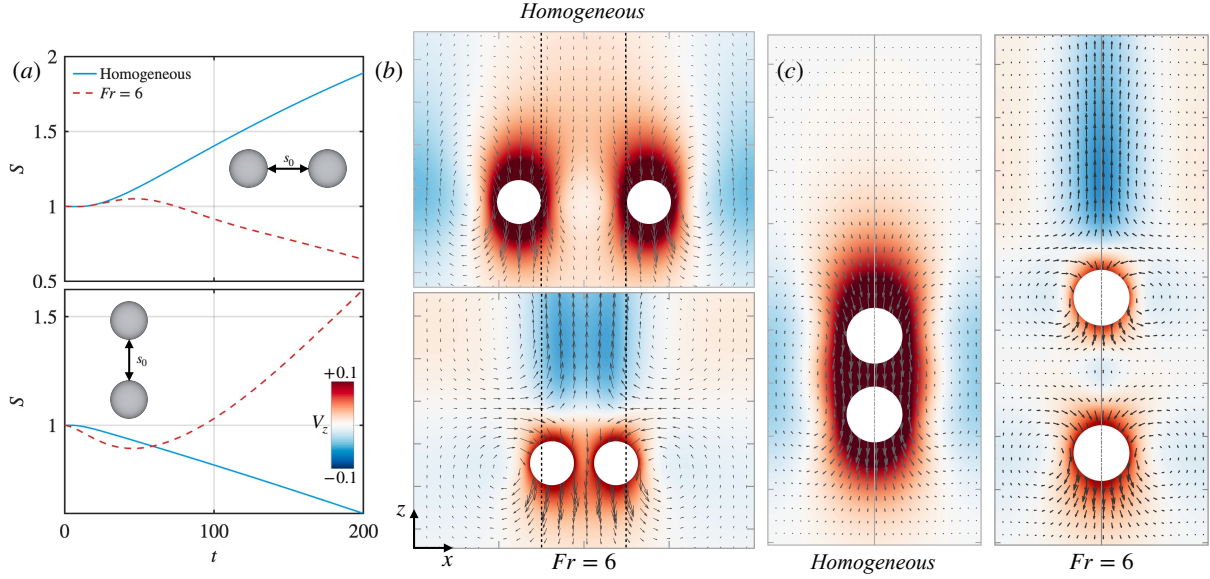


Figure 5.2: Panel (a) shows the time history of the surface-to-surface separation distance for a settling pair of spherical particles in a linearly stratified fluid, for both the SBS and in-line configurations. For comparison, results are also shown for the corresponding cases in a homogeneous ambient. The non-dimensional parameters for the stratified cases were $Ar = 4.65$, $Fr = 6$ and $Sc = 700$. Panels (b) and (c) present qualitative results for the two configurations before the particles reach the bottom of the domain.

where a and b are the polar and equatorial radii, respectively. A schematic of these axes for spheroids, together with a comparison to a sphere, is shown in panel (c) of Fig. 5.1. Unless stated otherwise, we consider oblate and prolate spheroids with $\mathcal{AR} = 1/3$ and $\mathcal{AR} = 3$, respectively. For a sphere ($\mathcal{AR} = 1$), the volume-equivalent diameter reduces to the particle diameter, so that $D_{eq} = D_p$. The centroid of the trailing particle is initially positioned at two particle diameters below the top of the domain. Unless otherwise stated, the leading particle's initial position is one equivalent particle diameter (from surface-to-surface) below the trailing particle ($s_0 = 1$), which can be seen in panel (d) of Fig. 5.1. The initial orientation of the spheroids is kept such that the major axis is normal to the direction of gravity. The spheroids always start from rest, and settle in a quiescent background fluid. A similar setup for spherical particles is adapted for the benchmark tests, where for the side by side configuration (SBS), the separation distance from surface-to-surface is also set to $s_0 = 1$.

We perform highly-resolved numerical simulations of the governing equations in a three-dimensional rectangular Cartesian domain with dimensions $L_x \times L_y \times L_z = 12D_{eq} \times 12D_{eq} \times 24D_{eq}$, as shown in panel (b) of Fig. 5.1. The computational domain is divided into parallel subdomains, which are each uniformly discretised by a $64 \times 64 \times 32$ finite-

difference mesh. Unless otherwise stated, the mesh size used in this study is $384 \times 384 \times 768$, which corresponds to a resolution of $D_{eq}/\Delta x = 32$. This domain size is used throughout, unless stated otherwise. This resolution is sufficient to accurately capture the particle settling velocity and the transient jet dynamics, as confirmed by tests conducted at a lower resolution of $D_{eq}/\Delta x = 20$ with less than 3% variation in particle settling velocity (not presented herein). Periodic boundary conditions are applied on the side boundaries, and the velocity boundary condition at the top and bottom boundaries correspond to free slip and no-penetration. The global mesh contains approximately 1.13×10^8 grid points and is decomposed into 864 parallel subdomains. Representative spheroid-pair simulations were advanced for $\mathcal{O}(10^5)$ time steps using 864 parallel processes distributed over 16 CPU compute nodes and required approximately four days of wall-clock time.

5.2 Benchmark tests

Building on Chapter 4, which presented benchmark tests for isolated spherical particles settling in both homogeneous and density-stratified fluids, this section reports benchmark results for two interacting spherical particles in a density-stratified fluid. For these tests, we consider two ambient density profiles: a linearly stratified background and a sharply stratified background. Let us first consider a linearly stratified background and draw qualitative comparisons with the results of Doostmohammadi and Ardekani [46]. In panel (a) of Fig. 5.2, the time evolution of the surface-to-surface separation distance shows that stratification can qualitatively alter, and in some cases reverse, the interaction between the particles relative to a homogeneous ambient.

For the SBS configuration, the homogeneous case is characterised by an almost monotonic increase in the separation distance, indicating mutual repulsion between the particles. When a linear stratification is introduced, this behaviour changes markedly: the separation instead decreases with time, demonstrating an effective attraction that draws the particles together. This suggests that stratification modifies the surrounding flow and buoyancy field in a way that suppresses the mechanisms responsible for lateral repulsion in the homogeneous case. In the in-line configuration, the homogeneous ambient displays the opposite trend, with the separation distance decreasing as the trailing particle is drawn towards the leading particle, consistent with wake-induced drafting. In a linearly stratified ambient, however, the separation increases, indicating repulsion. Here, stratification alters the structure and influence of the leading-particle wake, reducing the tendency for the trailing particle to be entrained and instead promoting separation. Overall, Fig. 5.2

shows that stratification can switch the interaction from attraction to repulsion, or vice versa, depending on the particle arrangement.

These observations are consistent with the findings of Doostmohammadi and Ardekani [46] for a spherical particle pair settling in a linearly stratified fluid. It is noteworthy that, in a conference presentation, the experiments of Mercier et al. [167] reported that for moderate Fr the SBS configuration did not exhibit the attraction observed here. This highlights that the interaction dynamics depend sensitively on the underlying dimensionless parameters. A systematic determination of the parameter ranges over which these transitions occur is, however, beyond the scope of the present work.

When considering a sharply stratified fluid, comparisons are provided in panel (a) of Fig. 5.1 with the numerical study of Deepwell et al. [16]. In this case, the vertical extent of the domain is increased to $L_z = 30D_p$, similarly to Deepwell et al. [16], and the ambient density field is prescribed using an error-function profile,

$$\rho_f(z) = \rho_{f,0} + \frac{\Delta\rho}{2} [1 - \text{erf}(z/H)], \quad (5.3)$$

where $\rho_{f,0}$ and $\rho_{f,1}$ are the densities of the upper and lower layers, respectively, and $\Delta\rho = \rho_{f,1} - \rho_{f,0}$. The parameter H sets the thickness of the transition region, and we take $H = D_p$ in the present simulations as done in the work of Deepwell et al. [16].

Rather than using the Froude number to characterise the stratification strength in this configuration, we follow Deepwell et al. [16] and introduce the dimensionless density ratio Γ :

$$\Gamma = 1 - \frac{\rho_p - \rho_{f,1}}{\rho_p - \rho_{f,0}} = \frac{\rho_{f,1} - \rho_{f,0}}{\rho_p - \rho_{f,0}}. \quad (5.4)$$

With this definition, $\Gamma = 0$ recovers a homogeneous ambient ($\rho_{f,0} = \rho_{f,1}$), while $\Gamma = 1$ corresponds to a particle that is neutrally buoyant in the lower layer ($\rho_p = \rho_{f,1}$).

Panel (a) then compares the evolution of the relative configuration of the pair with the results of Deepwell et al. [16], focusing on the orientation angle ϕ between the line joining the particle centres and the vertical direction as Γ is varied. This provides a tight benchmark, since ϕ is sensitive to small differences in the hydrodynamic interaction between the particles as they approach and traverse the density transition. Alongside the quantitative comparison, the panel also includes a schematic of the problem setup and the associated definitions (adapted from Deepwell et al. [16]) to clarify the geometry and the meaning of ϕ and Γ .

To illustrate the interaction dynamics underlying the trends in ϕ , qualitative particle

configurations are also shown for two representative cases, $\Gamma = 0.1$ and $\Gamma = 0.5$, at $t = 6$ and $t = 30$. These snapshots highlight how changes in Γ modify the evolution of the pair over time. For all cases considered here, the particle Reynolds number based on the Stokes settling velocity was fixed at $Re = 1/4$, the Schmidt number was set to $Sc = 700$, and the initial orientation was prescribed as $\phi_0 = 67.5^\circ$. As shown in panel (a) of Fig. 5.1, the present simulations reproduce the trends reported by Deepwell et al. [16] for the evolution of the orientation angle ϕ over the range of Γ considered. After release, ϕ increases from its initial value, indicating that the pair rotates towards a SBS arrangement. This tendency becomes stronger as Γ is increased. The snapshots at $t = 6$ and $t = 30$ for $\Gamma = 0.1$ and $\Gamma = 0.5$ are consistent with this trend, showing a more pronounced lateral alignment of the pair at higher Γ .

Lastly, since most benchmark comparisons are performed for spherical particles, we also include a non-spherical case to assess the method for spheroidal geometries. Specifically, panel (d) compares the average settling velocity V_z of a pair of oblate spheroids with $\mathcal{AR} = 1/3$ against the numerical results of Ardekani et al. [41] for $Ar = 80$ in a homogeneous fluid. The particles are initially in a broadside-on configuration with an initial surface-to-surface separation of $s_0 = 1D_{eq}$. The comparison shows that the present simulations capture the settling velocity trend reported by Ardekani et al. [41].

5.2.1 Boussinesq approximation: Validation

A comparison of the settling dynamics predicted by the Boussinesq and non-Boussinesq formulations is provided in Fig. 5.3. An oblate spheroidal particle pair is considered, with $\mathcal{AR} = 1/3$, $Ar = 4.65$, $Fr = 8$, and $Sc = 700$. The settling velocity time histories of both the leading and trailing particles are in close agreement with the Boussinesq results, indicating that the two models give essentially the same outcome for the present parameters. Similar assessments have been reported for a spherical particle settling in a linearly stratified fluid by Doostmohammadi et al. [30] and for a spherical particle crossing a sharp density transition layer by Wang et al. [168]. In these salinity-stratified configurations (with $Sc \gg 1$), and small relative density variations, the Boussinesq approximation yields results that are indistinguishable from the corresponding non-Boussinesq predictions.

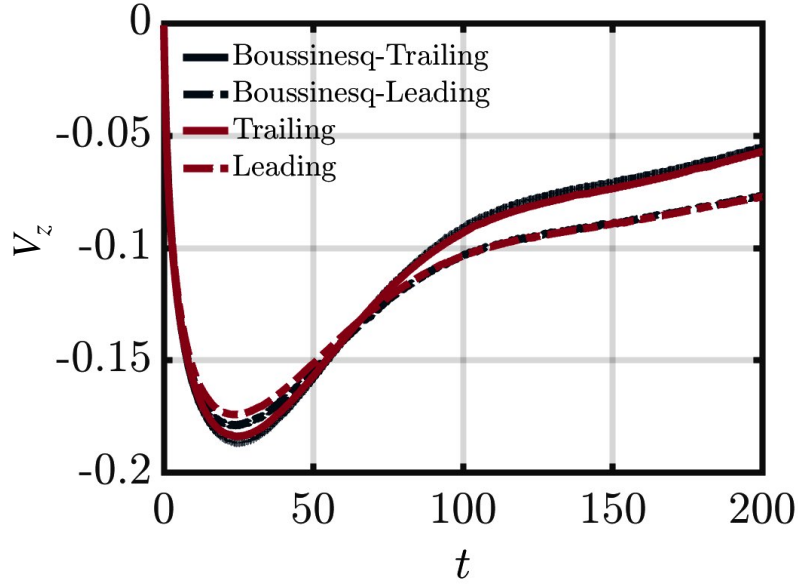


Figure 5.3: Time history of the settling velocity of an oblate spheroidal particle pair with $\mathcal{AR} = 1/3$, $Ar = 4.65$, $Fr = 8$, and $Sc = 700$, comparing simulations using the incompressible Navier-Stokes equations with the Boussinesq approximation and without the Boussinesq approximation.

5.3 In-line spheroids in a density-stratified fluid

In this section, we present the computational results of the pairwise interaction between an initially in-line pair of spheroidal particles settling in a linearly-stratified fluid. The investigation considers the effect of Fr on the interaction dynamics, while also considering the particle aspect ratios and the initial separation distance s_0 (panel (d) of Fig. 5.1). The particles are initially oriented ‘broadside-on’, which corresponds to when the major axis is normal to the direction of gravity, such that the polar angle θ made by the spheroid’s polar axis (a) with the z -coordinate is initially 0° (90°) for an oblate (prolate) spheroid (panel (c) of Fig. 5.1). We will use the term ‘edgewise-on’ to refer to when the particles’ major axis is aligned with the direction of gravity, such that the polar angle corresponds to 90° (0°) for an oblate (prolate) spheroid.

5.3.1 Settling behaviour

Let us first examine the settling dynamics of the particle pair by considering the effects of the background fluid density gradient when $Ar = 4.65$. In Fig. 5.4, panels (a) and (c) showcase the temporal evolution of the average velocity profiles when varying Fr for

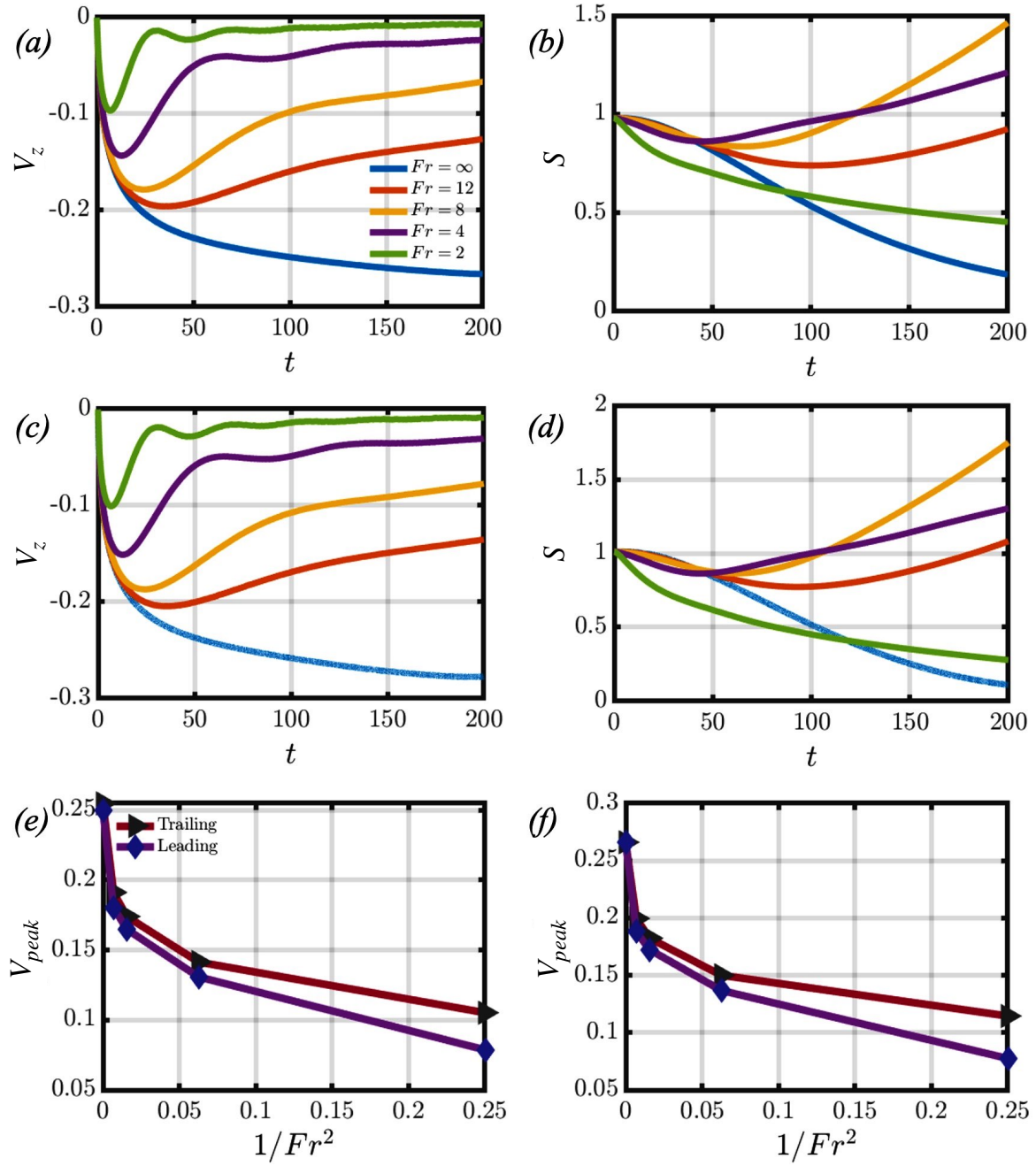


Figure 5.4: Panels (a) and (b) present the temporal evolution of the average settling velocity and the normalised distance between the particle surfaces for an oblate particle pair settling in a background fluid of different Fr . Panels (c) and (d) present the same results for a prolate particle pair. Panels (e) and (f) showcase the difference in peak velocities between the leading and trailing particles across different Fr for the oblate and prolate pairs, respectively.

oblate and prolate spheroids, respectively. The time-dependent average velocity profiles are calculated by

$$V_z = \frac{1}{2}(V_z^l + V_z^t), \quad (5.5)$$

where V_z^l and V_z^t refer to the settling velocities of the leading and trailing particles, respectively. In the case of a homogeneous fluid ($Fr = \infty$), the particles start from rest and accelerate until they attain a terminal velocity. The particles then continue to settle at that terminal velocity until reaching the bottom of the domain. However, in the case of a stratified fluid, the particles start from rest at a position where their density is greater than that of the surrounding fluid. The particles accelerate, and as the background fluid density increases, the buoyancy force acting on the spheroids will oppose their settling motion. Therefore, the particles attain a peak velocity, and the balance of drag and buoyancy forces causes the particles to decelerate.

When considering the effect of increasing the stratification strength (decreasing Fr), it can be seen in panels (a) and (c) of Fig. 5.4 that the average peak velocity decreases with Fr . This occurs because the effects of buoyancy more efficiently inhibit the settling motion of the spheroidal pair, and aligns with findings from other studies on particles settling in stratified fluids [30, 35, 169, 170]. Fig. 5.4 indicates that for both oblate (panel (e)) and prolate (panel (f)) spheroidal pairs, the gap in peak velocities between the leading and trailing particles grows as the stratification strength increases. Moreover, the trailing particle consistently attains a larger peak velocity. Panels (b) and (d) of Fig. 5.4 showcase the temporal evolution of the normalised distance (S) between the leading and trailing particles for oblate and prolate spheroids, respectively. In the homogeneous case, the particles tend to draft as they settle. This is due to the trailing particle being attracted into the wake of the leading particle, thus decreasing the distance between them.

In contrast to the case of larger Ar studied by Ardekani et al. [41], however, the two particles do not come in contact. This has also been tested by doubling the vertical extent of the domain to $48D_{eq}$ for the homogeneous cases, and no contact was found. When introducing stratification effects, it can be seen that the two particles draft initially at moderate stratification, then tend to separate. The drafting duration increases with Fr when considering $Fr \geq 4$. Post the drafting phase, the particles tend to separate such that their separation distance increases at later times when decreasing Fr . This observation is true for $Fr = 12$ and $Fr = 8$, but no longer remains valid at $Fr = 4$. Furthermore, when $Fr = 2$, it is found that the particles tend to draft and do not separate at later times. This reversal is attributed to the increased buoyancy force acting on the particle pair at lower Fr , which decreases the settling velocity of the spheroidal pair as previously observed.

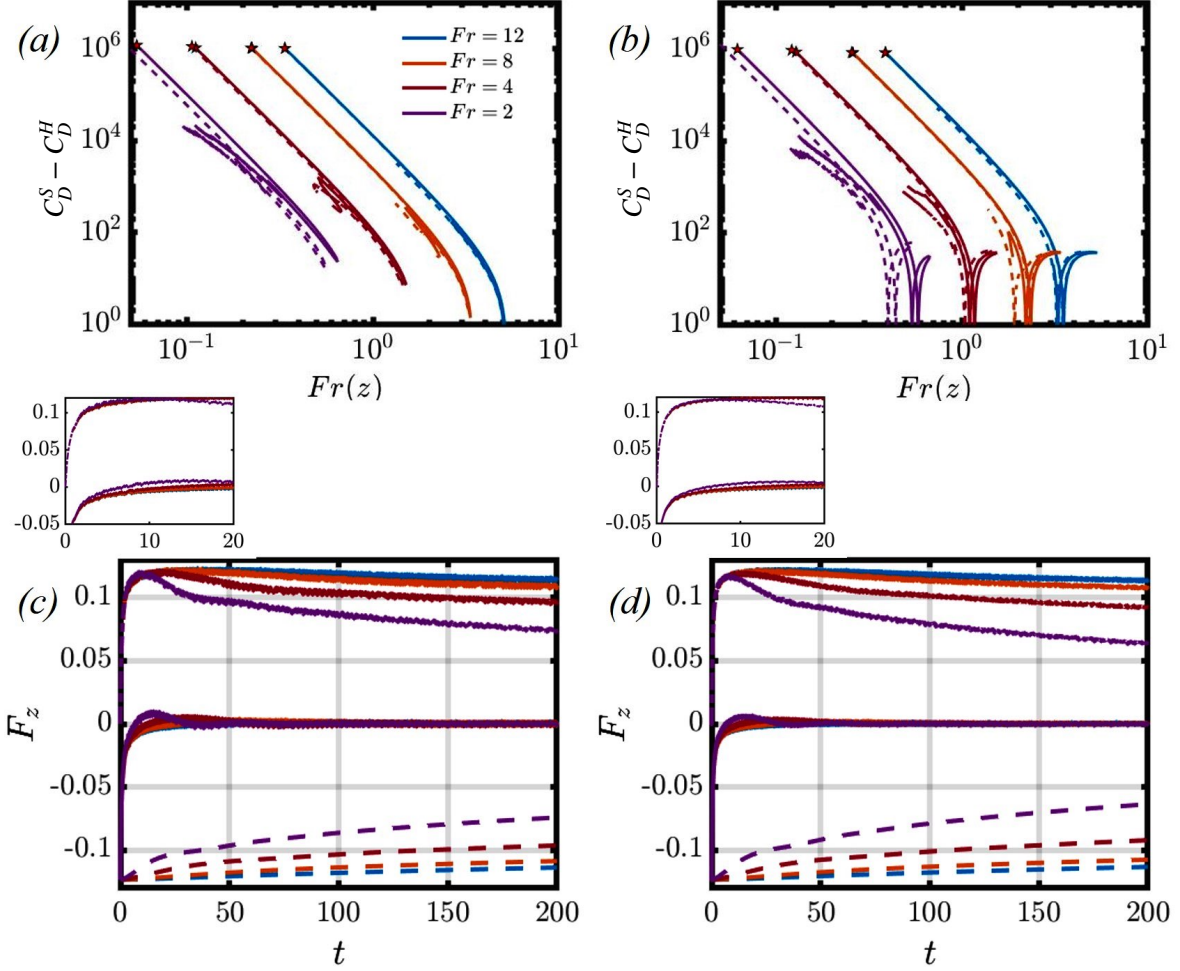


Figure 5.5: Difference between the stratification and homogeneous drag coefficients for different Fr for an oblate and a prolate spheroidal pair, shown in (a) and (b), respectively. The dashed and solid lines correspond to the leading and trailing particles, respectively. In panels (c) and (d), the temporal evolution of the buoyancy (dashed), net (solid), and hydrodynamic (dash-dotted) forces are plotted for an oblate and prolate pair, respectively.

A deeper exploration of the complexities behind these observations will be presented in Section 5.3.2.

The literature reveals that stratification significantly increases the drag experienced by a settling particle [30, 35, 37, 54]. If we consider the dynamics of a spheroidal particle settling due to gravity, the translation equation of motion can be written as

$$\rho_p \mathcal{V} \frac{d\mathbf{u}_p}{dt} = \rho_p \mathbf{g} \mathcal{V} - \int_{\mathcal{V}} \rho_f \mathbf{g} dV + \int_{\mathcal{S}} \boldsymbol{\tau} \cdot \mathbf{n} dS, \quad (5.6)$$

where $\boldsymbol{\tau} = -p\mathbf{I} + \mu(\nabla\mathbf{u} + \nabla\mathbf{u}^T)$ is the stress tensor. The first and second terms on the right-hand side account for the buoyancy force, and the third term accounts for the

hydrodynamic forces. Studies have shown that the added mass and history forces are negligible when compared to the buoyancy and hydrodynamic forces for a particle settling in a stratified fluid [30, 35, 37]. To measure the extent of drag due to stratification, we presume that the spheroid settles in a quasi-steady state and neglect the added mass and history forces. A stratification drag coefficient can be introduced as [54]:

$$C_D^S = \frac{4(\rho_p/\rho_f(z) - 1)gD_{eq}}{3V_z^2 \mathcal{AR}^\alpha}, \quad (5.7)$$

where $\rho_f(z)$ represents the unperturbed background fluid density profile, and V_z denotes the particle velocity at the particle position z . The parameter α is taken as $-2/3$ for an oblate spheroid, and $1/3$ for a prolate spheroid [41]. Furthermore, several different parameters may also be introduced as a function of the particle's position,

$$\Omega(z) = \rho_p/\rho_f(z), \quad (5.8)$$

$$Re(z) = \frac{|V_z|D_{eq}}{\nu}, \quad (5.9)$$

where $\Omega(z)$ is the density ratio, ν is the kinematic viscosity, and $Re(z)$ is the local Reynolds number. The local Froude number $Fr(z)$ may be defined as $\sqrt{Re(z)/Ri}$, where $Ri = \gamma g D_{eq}^3 / U \mu_f$ is the Richardson number.

Kishore and Gu [171] provide a drag coefficient for a spheroid settling in a homogeneous fluid (C_D^H), valid for $1 \leq Re_p \leq 200$ and $0.4 \leq \mathcal{AR} \leq 4$ with an error of less than $\pm 4\%$:

$$C_D^H = \frac{24\mathcal{AR}^{0.49}}{Re(z)} [1.05 + 0.152Re(z)^{0.687} \mathcal{AR}^{0.671}]. \quad (5.10)$$

Note that when $\mathcal{AR} = 1$, this equation corresponds to a modified form of the drag coefficient formula for spheres in a homogeneous fluid found by Schiller and Naumann [172].

In panels (a) and (b) of Fig. 5.5, the difference between the stratified and homogeneous drag coefficients is measured ($C_D^S - C_D^H$) when varying Fr for an oblate and prolate spheroidal pair, respectively. As seen by More et al. [35], the particles initially start from rest and accelerate, leading to an increase in $Fr(z)$. During the acceleration phase, the disparity between the stratified drag coefficient, C_D^S , and the homogeneous drag coefficient, C_D^H , diminishes, reaching its lowest point as the particles attain their maximum velocity. As the influence of buoyancy intensifies, the drag induced by stratification surges, causing the particles to slow down. The results show that the stratification drag coefficient is orders of magnitude larger than its homogeneous counterpart. The difference between

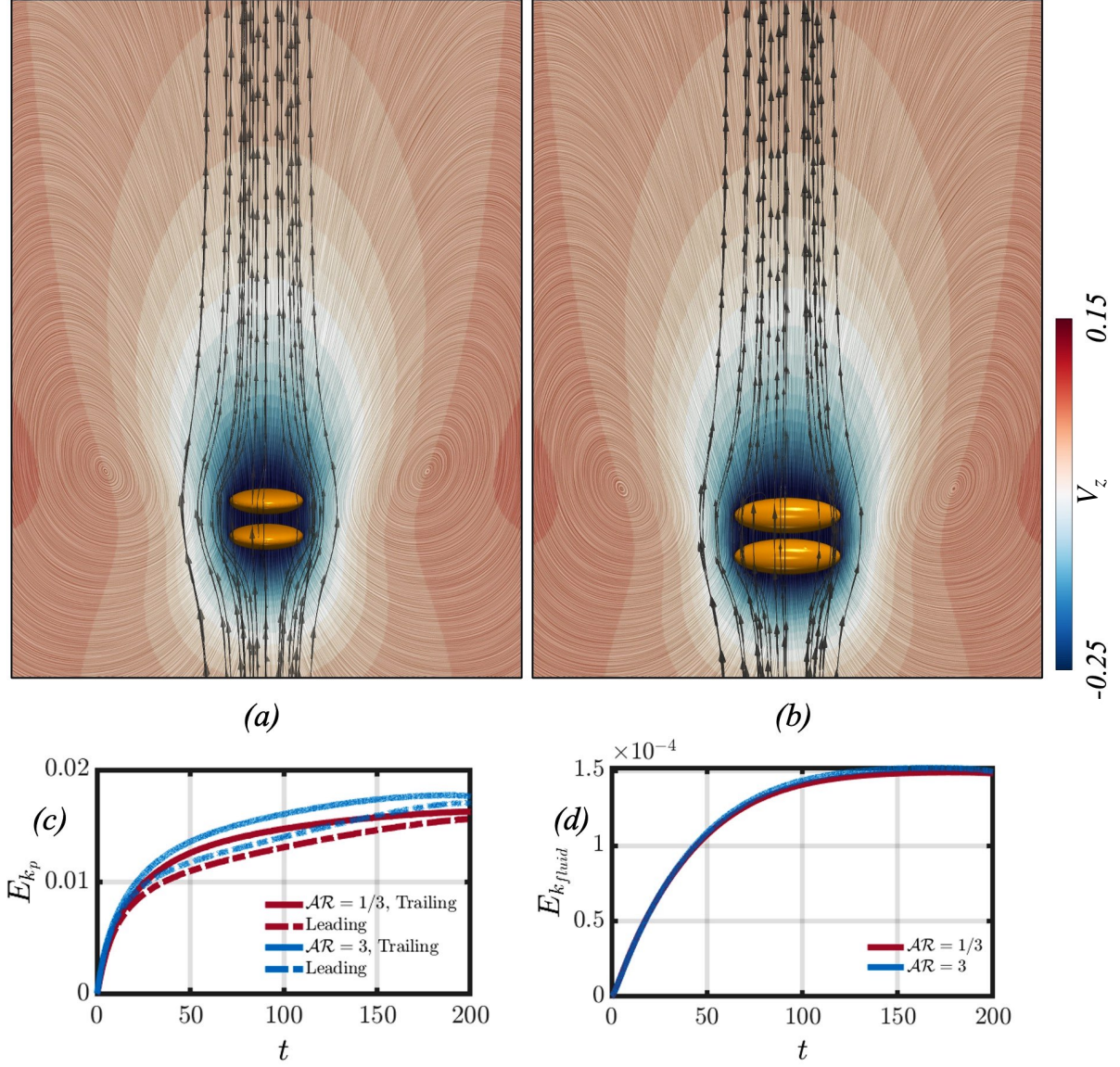


Figure 5.6: Panels (a) and (b) showcase the flow field for a pair of (a) oblate and (b) prolate particles settling in a homogeneous fluid, where the background colourmap depicts the z -velocity field. The background streamlines presented are in the stationary reference frame, and the streamlines are in the reference frame of the leading particle. Panels (c) and (d) showcase the time history of the particle and fluid kinetic energies, respectively. The particle and fluid kinetic energies are normalised by their respective masses (MU^2).

the two drag coefficients reveals the importance of accounting for the additional drag due to stratification when studying particulate transport in fluids with density gradients.

In panels (c) and (d) of Fig. 5.5, the buoyancy (dashed lines), hydrodynamic (dashed-dotted lines), and net force (solid lines) acting on the trailing particle are measured for different Fr for the oblate and prolate cases, respectively. The buoyancy and hydrodynamic forces are calculated using Eq. 5.6, and the net force is taken as the sum of the two contributions. In a homogeneous fluid, the buoyancy force remains constant and can be determined by $F_B = (\rho_p - \rho_{f,0})g\mathcal{V}$. As the particle accelerates over time and reaches its peak velocity, a balance is established between the hydrodynamic forces and the buoyancy force, and the particle settles at this constant terminal velocity.

In contrast, within a stratified fluid, the initial magnitude of the buoyancy force is greatest since the disparity in density between the particle and the surrounding fluid is at its maximum. This creates a negative net force at the outset, prompting the particle to accelerate. As the particle accelerates, hydrodynamic forces build up, and the magnitude of the buoyancy force diminishes. The particle's peak velocity is achieved when the hydrodynamic force exceeds the buoyancy force. At this point, the buoyancy force is insufficient to offset the hydrodynamic force, leading to the particle's deceleration when the net force becomes positive. If the particle reaches a position where it is neutrally buoyant, its settling motion will stop, as there is no longer any net force acting on it.

5.3.2 Flow field and particle dynamics

This section will build upon the findings of Section 5.3.1, and investigate the details of the flow field, particle orientation, and interaction between the particles when $Ar = 4.65$.

Let us first consider the interaction between spheroids settling in a homogeneous fluid. Panels (a) and (b) of Fig. 5.6 showcase the flow fields for an oblate and prolate spheroidal pair settling in the absence of stratification, respectively. The analysis of the flow fields indicates that the settling behavior of the spheroidal particle pair is axisymmetric, featuring areas of negative velocity in the fluid surrounding the particles. In panels (c) and (d), the kinetic energy for both the particle pair and the surrounding fluid is depicted. The total kinetic energy E_k of the system is defined as follows,

$$E_k = \frac{1}{2}\rho_0 \int_V (u^2 + v^2 + w^2) dV, \quad (5.11)$$

and may be separated into two different contributions. The two contributions are the

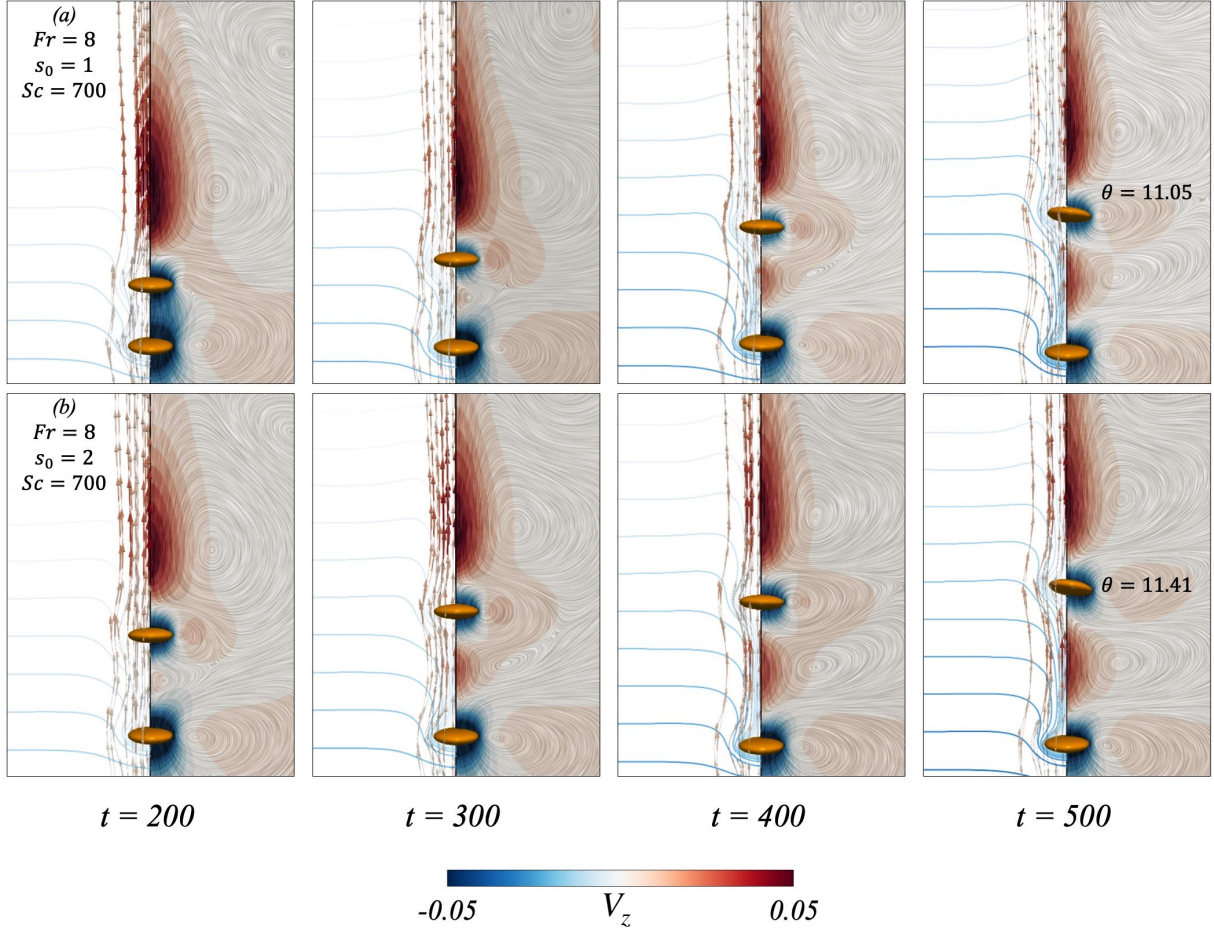


Figure 5.7: Results for the dynamic interaction between two settling oblate spheroids under different conditions. From left to right of every row, each panel showcases the flow field (right side) and streamlines (left side) in the reference frame of the leading particle. The left side of each panel also presents contours depicting the distortion of the pycnoclines, which are coloured such that the dark blue represents a heavier fluid. The difference in density between two adjacent pycnoclines is $\Delta\rho_f/\gamma D_{eq} = 1.14$. The colour map in the flow field illustrates the fluid velocity. Rows (a-b) correspond to $(Ar, \mathcal{AR}, Fr, s_0) = (4.65, 1/3, 8, 1), (4.65, 1/3, 8, 2)$, respectively.

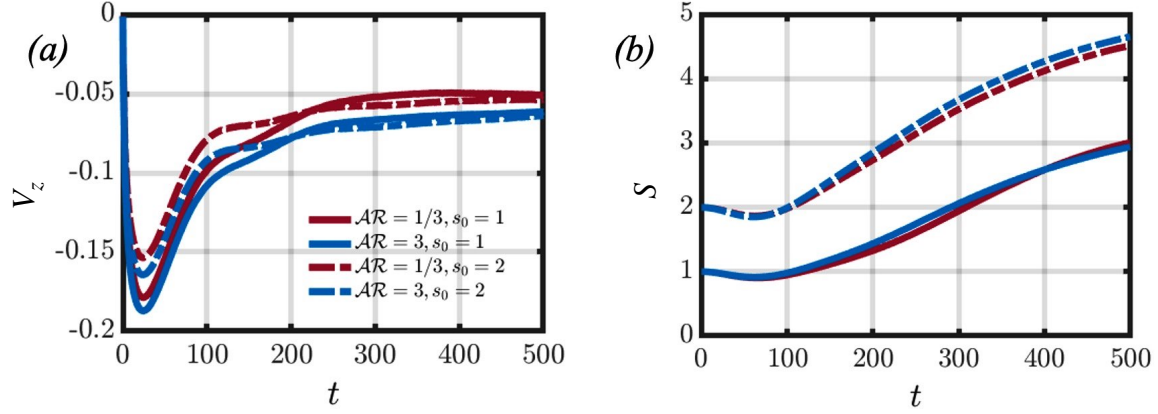


Figure 5.8: This figure showcases the settling dynamics (a-b) when varying s_0 for both an oblate and prolate particle pair. The results showcase the normalised settling velocities and separation distances between the two spheroids.

kinetic energy of the particles and the background fluid, such that $E_k = E_{k_p} + E_{k_{fluid}}$. It is observed that the kinetic energy associated with the trailing particle is greater than that of the leading particle at later times. This difference is attributed to the pressure gradient induced by the leading particle's wake, which propels the trailing particle to higher settling velocities. As for the fluid's kinetic energy, it increases until reaching a steady state, signifying that the particle pair has reached a constant terminal velocity.

When considering the flow field for an oblate spheroidal pair settling in a stratified fluid, Fig. 5.7 showcases the flow field at different times for two cases. These two cases correspond to a base case with $(Fr, s_0, Sc) = (8, 1, 700)$ in row (a), and increasing the initial separation distance in row (b). When the spheroids settle in a stratified fluid, they drag along with them lighter fluid which affects their settling velocities as seen in Section 5.3.1. The dragged fluid can be visualised by the distortion of the pycnoclines on the left-hand side of each panel. This fluid moves along the trailing spheroid until it reaches its rear stagnation point, where it forms an upward jet that returns this light fluid to its neutrally buoyant position [11]. The upward jet can be identified as the region with positive velocity (coloured in red) in Fig. 5.7. At $t = 200$, it can be seen in row (a) that the fluid neighboring the particle has a negative velocity. In time, the two particles separate due to viscous dissipation more efficiently limiting the inertial effects at this Ar number, such that the particles do not come in contact [46]. As the particles separate, the fluid region of negative velocity between the leading and trailing particles diminishes as seen at $t = 300$. The dragged lighter fluid by the leading particle then forms an upward jet in the region between the particle pair, further increasing the separation distance between the leading and trailing particles as seen in panel (b) of Fig. 5.8. This causes a sharp decrease

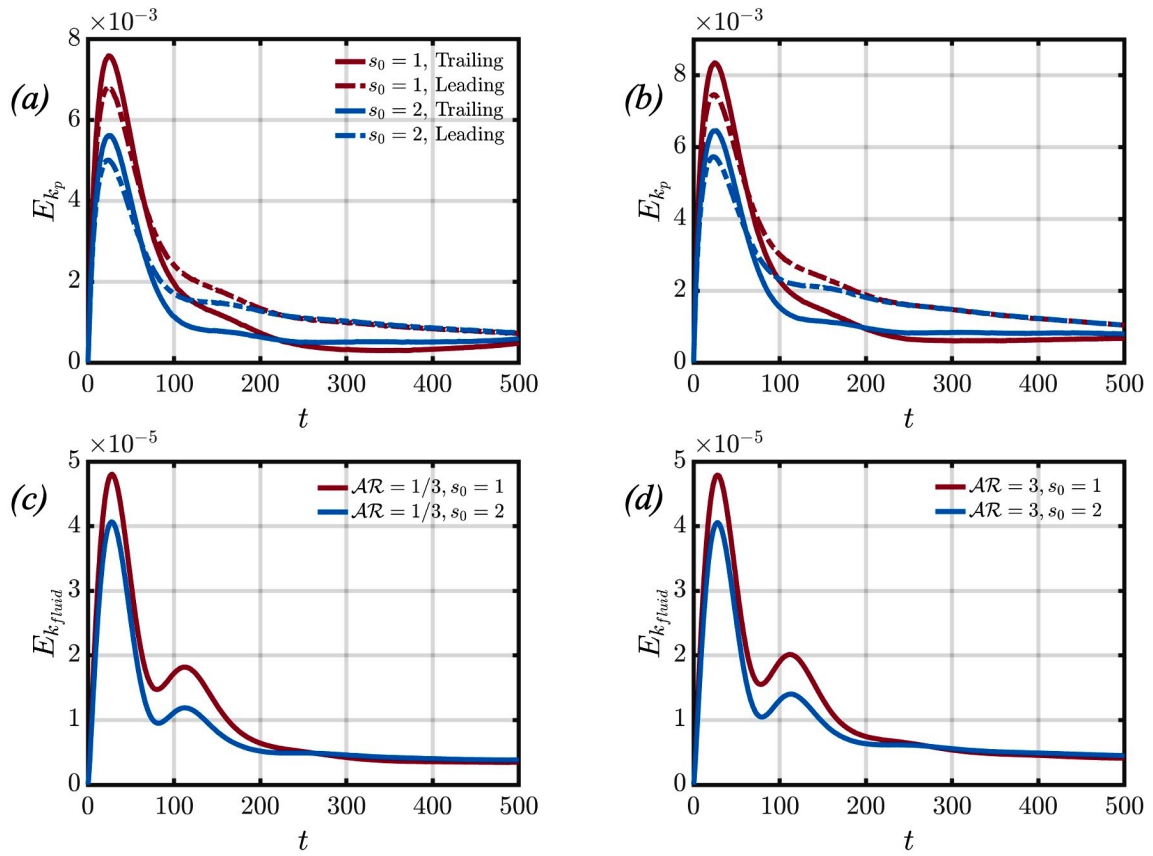


Figure 5.9: This figure showcases the particle and fluid kinetic energies when varying the initial separation distance for an oblate (panels (a) and (c)) and prolate (panels (b) and (d)) particle pair.

in the trailing particle's settling velocity, as seen in panel (a) of Figs. 5.8 and 5.9. More et al. [35] and Mercier et al. [37] have found that an oblate spheroid or disc settling in a stratified fluid reorients to its edgewise orientation when the particle's velocity decreases below some threshold value. In row (a) of Fig. 5.7, at the last time step, it can be seen that the trailing particle begins to reorient to its edgewise orientation, where $\theta \approx 11^\circ$.

In panel (b) of Fig. 5.7, the effect of increasing the initial separation distance between the two particles is considered. At the initial time step, the leading particle is surrounded by fluid that is heavier when compared to the base case. As a result, the leading particle is subjected to a larger buoyancy force, which limits its attainable peak velocity, as seen in panel (a) of Fig. 5.8. The decrease in peak velocity leads to a subsequent decrease in peak particle and fluid kinetic energies, as found in panels (a) and (c) of Fig. 5.9. However, a similar flow structure is found when compared to the base case ($s_0 = 1D_{eq}$), however at $t = 200$, the region of negative fluid velocity between the particle pair is no longer present. This can be explained by the wake of the leading particle causing a smaller pressure difference between the front and back of the trailing particle, such that the trailing particle's enhanced acceleration is not as significant when compared to the base case. This can be seen by the slightly decreased drafting time between the two cases (panel (b) of Fig. 5.8) and narrows the gap between the peak kinetic energies of the leading and trailing particles, as seen in panel (a) of Fig. 5.9. The trailing particle's kinetic energy then decreases, which increases the separation distance between the particle pair. The onset of the upward jet in the region between the particle pair can be found at earlier times ($t = 300$). As the trailing particle's velocity decreases, it starts to reorient to its edgewise orientation, as seen in the base case.

When considering a prolate particle pair settling in a stratified fluid, Fig. 5.10 considers the same study of varying the initial separation distance on the pairwise interaction. The overall flow dynamics are found to be similar to the oblate counterpart. There are a few subtle differences, however, that are worth mentioning. Firstly, the upward jet that forms behind the trailing particle, Fig. 5.10 shows that the jet radius is slightly larger when compared to the previous case. The particle settling velocities, found in panel (a) of Fig. 5.8 are slightly larger, leading to an increase in the particle kinetic energies (panel (b) of Fig. 5.9). The increase in particle kinetic energy compared to the oblate counterpart was also found for the homogeneous case, as seen in panel (c) of Fig. 5.6. Lastly, the reorientation of the trailing particle is not as significant when considering a prolate particle pair, as the polar angle varies by about $2^\circ - 3^\circ$ at $t = 500$, compared to $\theta \approx 11^\circ$ for the oblate case.

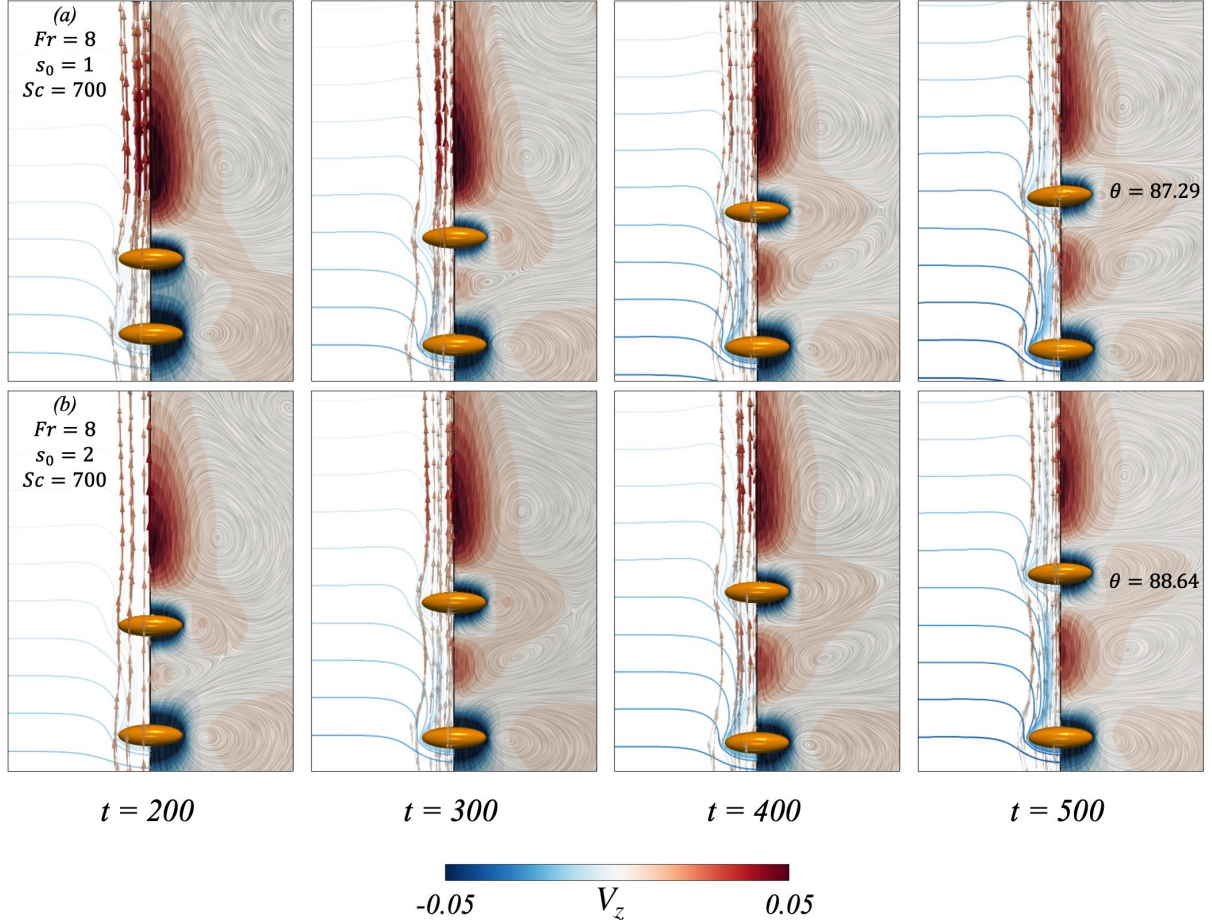


Figure 5.10: Results for the dynamic interaction between two settling prolate spheroids under different conditions. From left to right of every row, each panel showcases the flow field (right side) and streamlines (left side) in the reference frame of the leading particle. The left side of each panel also presents contours depicting the distortion of the pycnoclines, which are coloured such that the dark blue showcases a heavier fluid. The difference in density between two adjacent pycnoclines is $\Delta\rho_f/\gamma D_{eq} = 1.14$. The colour map in the flow field illustrates the fluid velocity. Rows (a-b) correspond to $(Ar, \mathcal{AR}, Fr, s_0) = (4.65, 3, 8, 1), (4.65, 3, 8, 2)$, respectively.

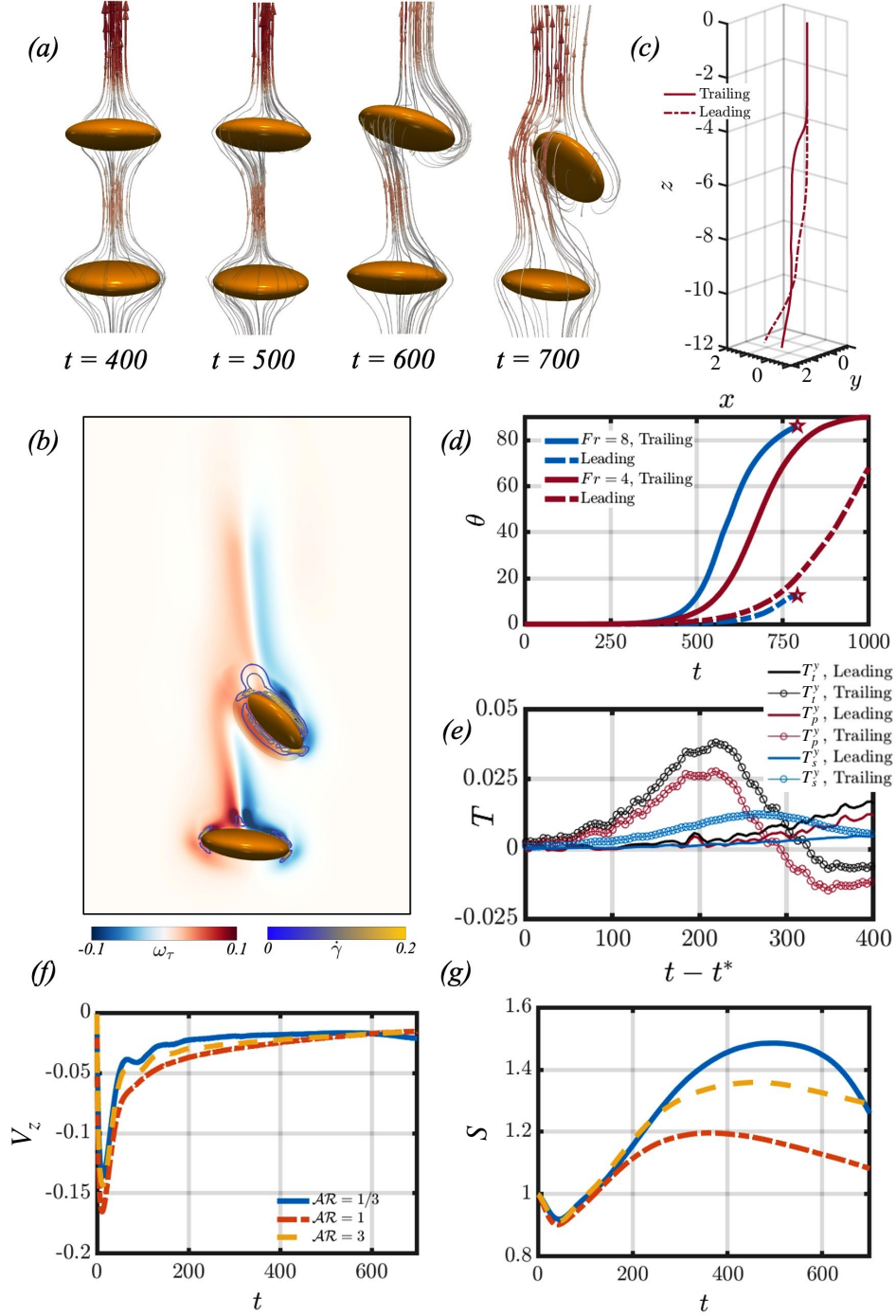


Figure 5.11: Panel (a) of this figure shows the evolution of the asymmetric side escape of the trailing particle for an oblate spheroidal pair when $Fr = 4$. At $t = 700$, panel (b) showcases the baroclinic vorticity contribution and contours of the shear rate near the particle surface. In panel (c), the three-dimensional trajectories of the trailing and leading particles are depicted, and panel (d) showcases the temporal evolution of the polar angle θ for two different Fr for an oblate spheroidal pair. Note that the pentagram in panel (d) is for the simulation end time. Panel (e) shows the evolution of the torques acting on the leading and trailing particles when $Fr = 4$. Panels (f) and (g) showcase the settling dynamics when $Fr = 4$ and varying the aspect ratio.

In Section 5.3.1, we have mentioned that in time, the separation distance between the two particles tends to increase when decreasing Fr . Here, we will examine the effect of decreasing Fr on the settling behaviour. In panel (a) of Fig. 5.11, the temporal evolution of the streamlines in the reference frame of the leading particle is presented for an oblate spheroidal pair when $Fr = 4$. At $t = 400$, the separation distance between the two particles is large, as seen in panel (g) of Fig. 5.11. However, axial symmetry breaks, and the trailing particle tilts clockwise as seen at $t = 500$. At this point, the trailing particle stands in the wake of the leading particle with its major axis tilted, which distorts the flow in the gap region between them. The flow grows increasingly asymmetric in this region at $t = 600$, and this asymmetry induces a slight clockwise tilt on the leading particle. The trailing particle then drifts laterally, starting to escape the wake of the leading particle. The separation distance between the particles then decreases, as the trailing particle attains its edgewise orientation. This phenomenon is reminiscent of the asymmetric side escape regime found for two in-line rising bubbles studied by Zhang et al. [63]. The three-dimensional trajectory of the leading and trailing particles can be appreciated in panel (c), and panel (d) showcases the time history of the polar angle θ for an oblate spheroidal pair settling when $Fr = 4$ and $Fr = 8$. Note that when $Fr = 8$, the simulation was stopped when the leading particle reached the bottom boundary, which corresponds to $t \approx 750$. The distortion of the isopycnals as the particles settle gives rise to baroclinic vorticity generation due to the misalignment of the density gradient with the direction of gravity. At $t = 700$, the vorticity field is depicted in panel (b) of Fig. 5.11. Closer to the particle surface, the formation of these vortices induces a high shear rate $\dot{\gamma} = \sqrt{2\mathbf{D} : \mathbf{D}}$, where $\mathbf{D}$ is the rate of strain tensor [39]. Furthermore, the total torque experienced by the spheroids as they settle is composed of two distinct components: the contributions from pressure forces and viscous stresses:

$$T_p = - \int_S (\mathbf{r} - \mathbf{r}_c) \times (p\mathbf{n}) dS, \quad (5.12)$$

$$T_s = \int_S (\mathbf{r} - \mathbf{r}_c) \times \mu(\nabla\mathbf{u} + \nabla\mathbf{u}^T) \cdot \mathbf{n} dS, \quad (5.13)$$

where $\mathbf{r} - \mathbf{r}_c$ indicates the distance from the particle surface to its centroid. The total torque can then be written as the sum of these two components, such that $T_t = T_p + T_s$. The temporal evolution of the different torque contributions when $Fr = 4$ can be found in panel (e), where $t^* \approx 400$ denotes the start of the trailing particle reorientation process. Concentrating on the y -component of the torque, the initial reorientation of the trailing particle is primarily driven by torque resulting from pressure forces. Yet, as the trailing particle narrows the gap distance and attains its edgewise orientation, baroclinic vortices

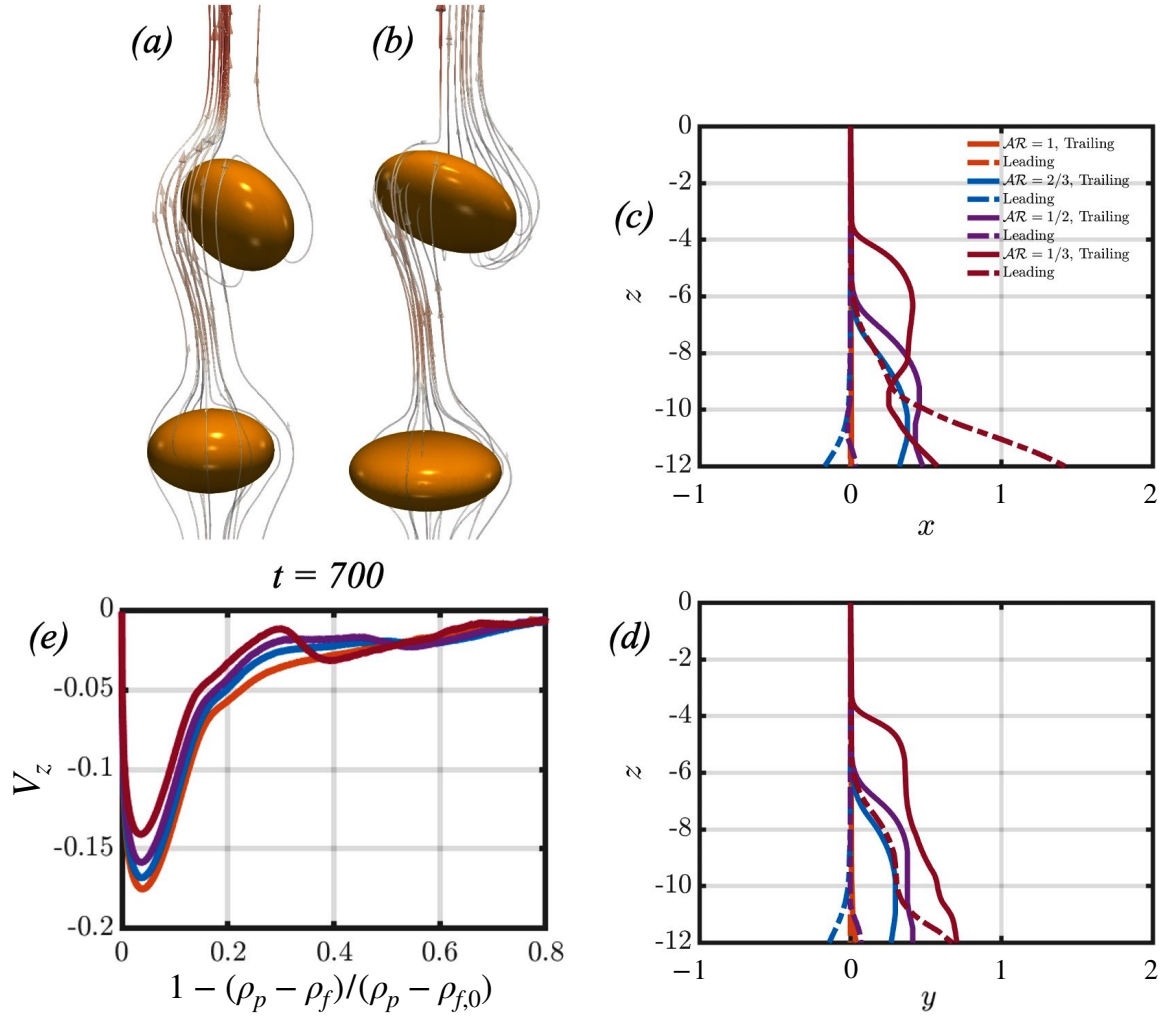


Figure 5.12: Panels (a) and (b) showcase the asymmetric side escape of the trailing particle when $Fr = 4$ for two different aspect ratios of oblate spheroids. The aspect ratios are $AR = 2/3$ and $AR = 1/2$, respectively. Panels (c) and (d) showcase the side views of the settling trajectories of the particle pair when varying AR and $Fr = 4$. Panel (e) showcases the evolution of the trailing particle's velocity profile when varying AR against the normalised density.

intensify, which amplifies the shear stress across its surface. The increase in the shear stress along the particle's surface gives rise to T_s , which opposes the decreasing pressure-induced torque contribution. When the particle slows down and reaches a stable edgewise orientation, the contribution from viscous torque decreases, leading to a reduction in particle rotation. A similar analysis can be made for the leading particle.

In Fig. 5.10, we can see that the induced reorientation of the trailing prolate particle is not as significant as the oblate counterpart, however, the trailing particle is found to tilt in the anticlockwise direction instead. When decreasing Fr , panels (f) and (g) of Fig. 5.11 provide a comparison of the average settling velocities and separation distances for three different aspect ratios. These aspect ratios correspond to the oblate spheroidal pair, prolate spheroidal pair, and a pair of spheres ($\mathcal{AR} = 1$). When considering $\mathcal{AR} = 3$ and $\mathcal{AR} = 1$, the decrease in distance between the leading and trailing particles when $t \geq 400$ is not as significant as the oblate counterpart. This can be explained by the reduced reorientation found earlier for the prolate particle pair, such that the decrease in separation distance is primarily due to buoyancy leading to a decrease in the leading particle's settling velocity.

Fig. 5.12 investigates the effect of gradually decreasing the aspect ratio on the trailing particle's escape when $Fr = 4$. Two additional aspect ratios are considered, and they are $\mathcal{AR} = 2/3$ and $\mathcal{AR} = 1/2$. The streamlines at $t = 700$ for these two cases can be found in panels (a) and (b) respectively. In both cases, the trailing particle is found to rotate clockwise, inducing an asymmetric flow pattern in the gap region between the two particles. When considering the settling trajectories, panels (c) and (d) provide a side view of the particle pair when varying $\mathcal{AR}$. For $\mathcal{AR} = 1$, the particles are seen to settle in line without colliding, as found at low Ar by Doostmohammadi and Ardekani [46]. As $\mathcal{AR}$ decreases, two main observations are made. When decreasing $\mathcal{AR}$, the magnitude of lateral drift of the trailing particle increases and occurs at a higher vertical position. This can be seen by investigating the side view of the particle trajectories. When considering the settling velocities of the trailing particles, panel (e) shows the evolution of the velocity profile as a function of the normalised density, where the magnitude of the peak velocity was found to increase with increasing $\mathcal{AR}$.

5.3.3 Role of Sc

Hanazaki et al. [173] and Yick et al. [54] examined how the Schmidt number influences the wake (or jet) structure in stratified flows. Their results indicate that increasing Sc

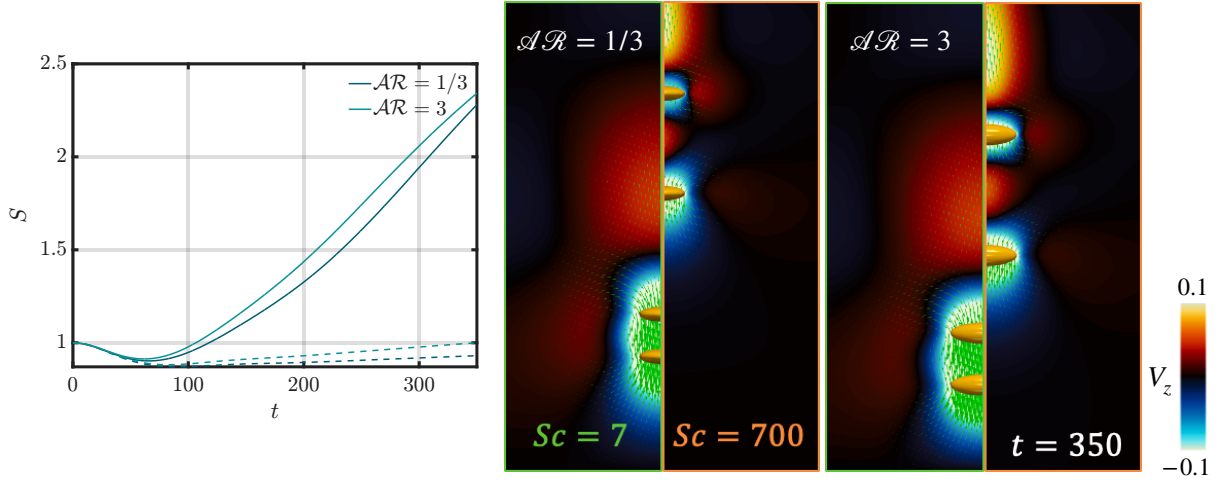


Figure 5.13: This figure shows the comparison in the separation distance S and the flow field at $t = 350$ when $Sc = 7$ (dashed lines) and $Sc = 700$ (solid lines) for oblate and prolate particles when $Ar = 4.65$ and $Fr = 8$.

leads to a thinner wake and a larger vertical velocity magnitude. For fixed stratification strength and Ar , the drag generally increases with Sc , which has been attributed to both the increase in wake velocity (thus baroclinic torque) and the reduction of pressure in the rear region of the particle [11, 32].

Fig. 5.13 illustrates these effects for an oblate ($\mathcal{AR} = 1/3$) and a prolate ($\mathcal{AR} = 3$) spheroidal particle pair at $Ar = 4.65$ and $Fr = 8$, comparing $Sc = 7$ (dashed lines) with $Sc = 700$ (solid lines). When Sc is decreased to 7, the wake behind the trailing particle becomes broader and the upward velocity magnitude decreases, consistent with the flow snapshots at $t = 350$. In this case, the particles remain close to one another for a longer time and the separation distance S grows more slowly than for $Sc = 700$, resulting in a smaller separation between the two particles induced by the flow field in the gap region between the two particles after the initial drafting phase. Furthermore, at low Sc the reduction in the trailing particle's settling velocity is limited, consistent with the weaker upward jet and a reduced pressure deficit in the rear region compared with $Sc = 700$. Finally, within the domain size considered here, no asymmetric side escape (and associated reorientation) of the trailing particle was observed when decreasing Sc .

5.3.4 Crossing the density transition

While in a linearly stratified fluid, particles settling due to gravity do not achieve a statistically steady state because of the continuously increasing background fluid density, an asymmetric side escape of the trailing particle at moderate stratification strengths

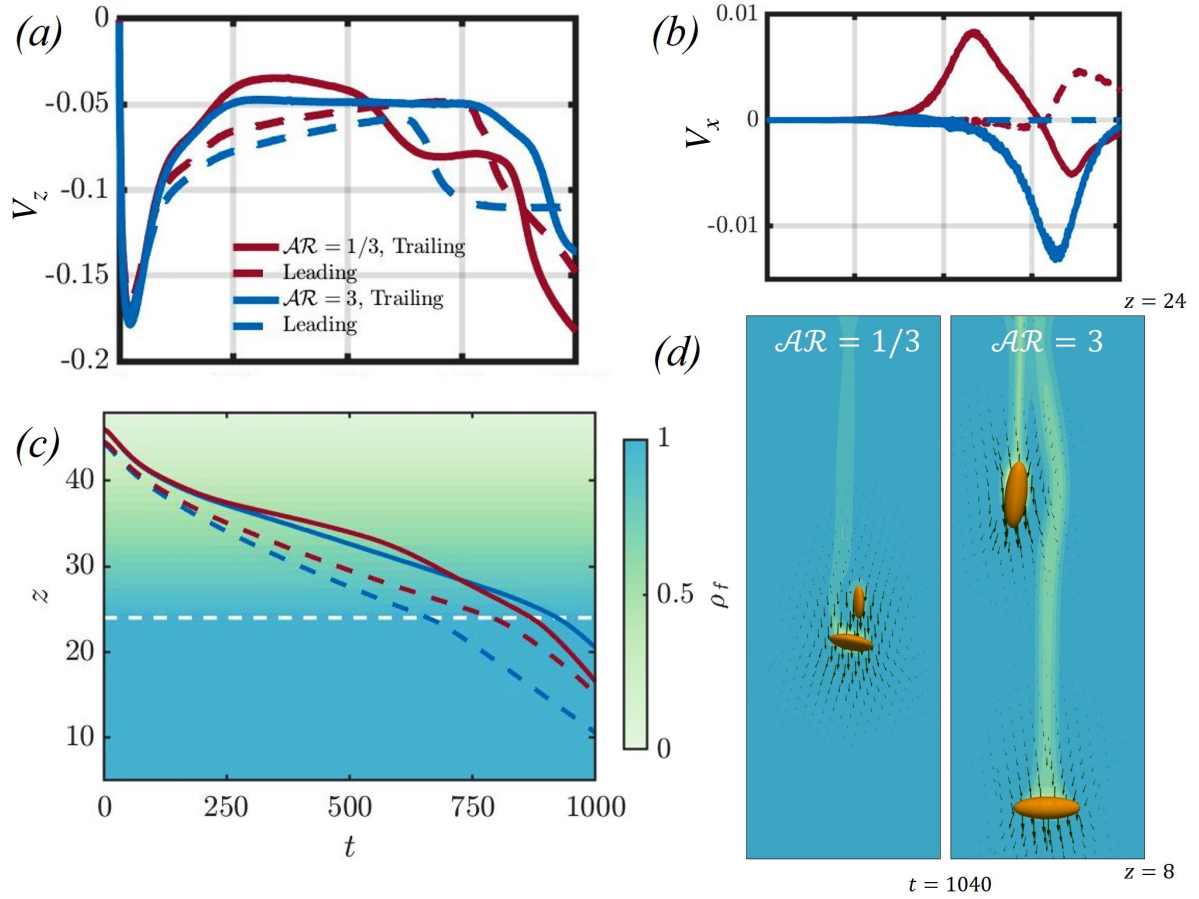


Figure 5.14: This figure showcases the transient dynamics of an oblate and prolate spheroidal pair settling in a linearly stratified fluid with $Fr = 8$, $Sc = 700$, and $Ar = 4.65$ for a vertical distance of $z = 24$, and settling in a fluid with constant density after that for a distance of $z = 24$. Panels (a) and (b) present the z and x particle velocities, and panel (c) showcases the temporal evolution of the vertical position of the spheroidal pair. The dashed white line in panel (c) is at $z = 24D_{eq}$, which is at the transition from linearly stratified above the line to constant density below the line. In panel (d), qualitative results are presented for the two cases after the particles cross the linearly stratified region at $t = 1040$.

is presented in this work. Previous studies have shown that the reorientation of discs settling in stratified fluids diminishes as they pass through the stratification interface [38]. Conversely, for prolate spheroids, Doostmohammadi and Ardekani [39] found that as a particle crosses a sharp density interface, it experiences enhanced reorientation to a broadside-on orientation, which diminishes once the particle settles into the denser fluid. Given that the reorientation of the particles past the density interface remains an open question for the specific configuration studied in this work, we include two additional cases to examine the effects of an extended domain on the reorientation and repositioning of these particles. Specifically, we will consider a linearly stratified fluid over a vertical height of $24D_{eq}$, followed by a region of constant fluid density extending another $24D_{eq}$ below the stratified layer. In Fig. 5.14, we present the (a) settling and (b) horizontal velocities of the particles as they traverse the linearly stratified region. As the particles exit the stratified zone, their settling velocities are expected to increase in magnitude as the lighter fluid column, drawn by the particles, returns to its neutrally buoyant state. Panel (c) illustrates the temporal evolution of the vertical position of the spheroidal particle pair, while panel (d) provides qualitative results for the particle pair at $t = 1040$. In panel (d), the figure presents a clip from $z = 8$ up to $z = 24$, where $z = 24$ denotes the vertical location below which the fluid density becomes constant. The full simulation domain extends to $z = 48$.

For an oblate particle pair, the trailing spheroid attains its edgewise orientation and continues to settle in that orientation beyond the density interface, with a larger settling velocity than the leading particle. The trailing particle also drifts closer to the leading particle, as indicated by the variation in V_x in panel (b). The leading particle maintains an orientation between broadside-on and edgewise-on ($\theta \approx 17.9^\circ$) during its descent past the stratified region. In contrast, for the prolate spheroidal pair, the leading particle continues to settle past the density interface in a broadside-on orientation, while the trailing particle attains an edgewise-on orientation. The separation distance between the particles is significantly larger compared to the oblate pair, which can be attributed to the increased settling velocity of the leading prolate particle due to its broadside-on orientation. It is important to note that these findings pertain to a particle pair settling in a stratified fluid with $Sc = 700$, corresponding to a salinity-stratified fluid, with particles having an equivalent spherical diameter of $250 \mu\text{m}$. The roles of Ar , Sc , and Fr are expected to have a non-trivial effect on the observed dynamics.

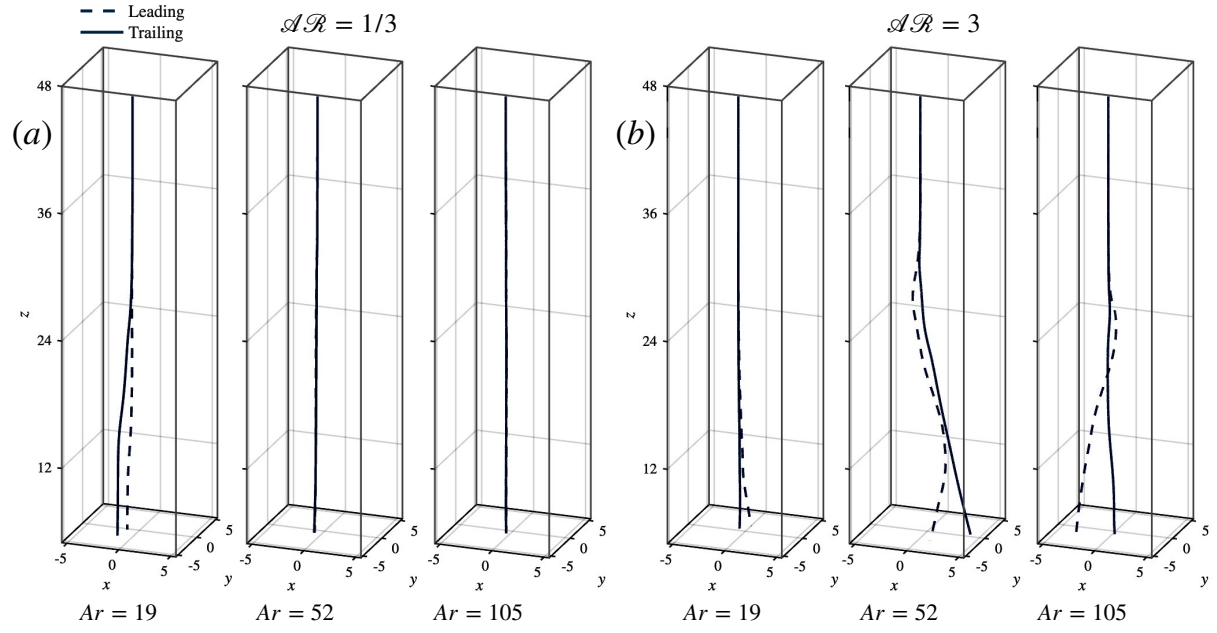


Figure 5.15: This figure shows the 3D trajectories of the leading and trailing particles when varying Ar and $\mathcal{AR}$. Here, $Fr = 8$, $Sc = 7$, and Ar is varied from 19 to 105.

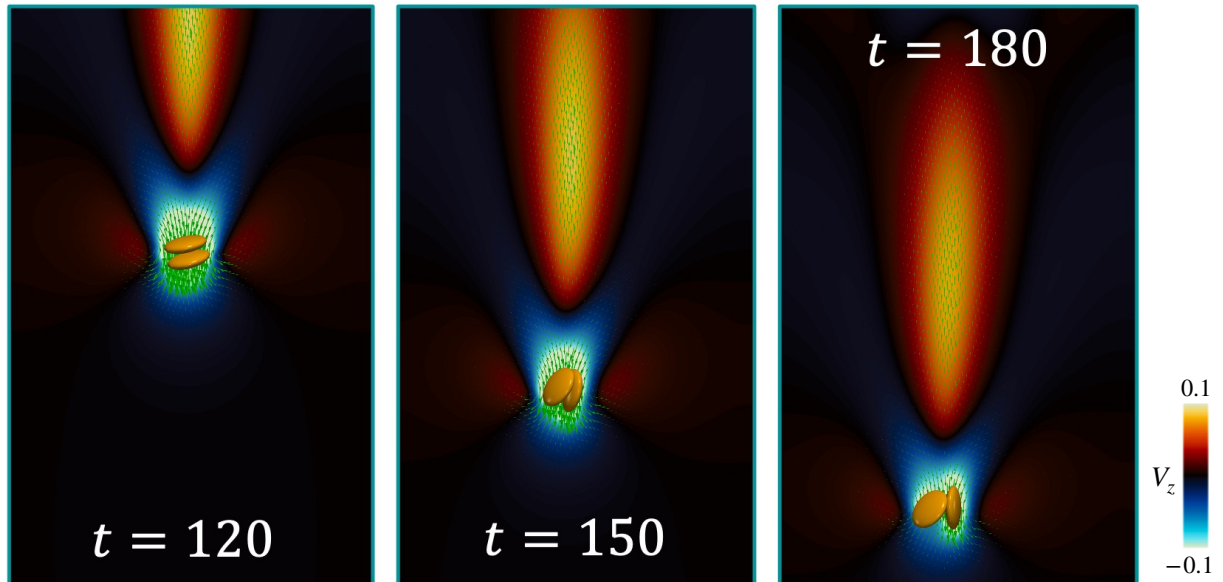


Figure 5.16: This figure shows the time history of the particle interaction when $\mathcal{AR} = 1/3$, $Ar = 19$, $Fr = 8$ and $Sc = 7$.

5.3.5 Role of Ar

In the previous sections, two distinct settling regimes were found, and these are the drafting-settling and asymmetric side escape regimes. However, the question remains: what happens to the settling dynamics when Ar increases? This section considers different Ar for both oblate $\mathcal{AR} = 1/3$ and prolate $\mathcal{AR} = 3$ spheroids settling in line when $Fr = 8$ and $Sc = 7$. To perform these simulations, a domain size of $12D_p \times 12D_p \times 48D_p$ is used, thus doubling the vertical extent of the domain. Furthermore, the mesh size utilised for these simulations is $384 \times 384 \times 1536$. The simulation setup in this section is the same as in Section 5.3.1, such that the particles start from rest and the initial separation distance between the two particles is equal to D_{eq} .

In Section 5.3.3, for an oblate spheroidal pair settling at low Ar and $Sc = 7$, the trailing particle initially drafts into the wake of the leading particle, without the formation of an upward jet in the gap region between the two particles. The particles do not come into contact and there is no significant reorientation of the particles. Increasing Ar leads to different settling regimes, similar to what is found by Ardekani et al. [41] in a homogeneous fluid. When $Ar = 19$, the trailing particle is seen to slither in the wake of the leading particle, so that the separation distance between the two particles decreases. As the particles approach one another at $Ar = 19$ and come in contact, or kiss, the particles start to reorient to their edgewise orientation at $t \approx 120$ as seen in Fig. 5.16. As they reorient, the trailing particle separates from the leading particle in the y -direction. The leading particle is seen to remain close to the centre of the domain, whereas the trailing particle separates as it attains its edgewise orientation.

In Fig. 5.15, the settling trajectories when $Ar = 52$ and $Ar = 105$ are also depicted. As seen when $Ar = 19$, the trailing oblate spheroid is seen to draft during its initial acceleration for both $Ar = 52$ and $Ar = 105$. The trailing and leading particles then come into contact, however, as opposed to $Ar = 19$, increasing the particle inertia leads to a new settling regime, where the oblate particle pair kiss and settle in-line until reaching the bottom boundary. This can be seen by the three-dimensional trajectories of the leading and trailing particles. In a homogeneous fluid, an isolated settling oblate particle in a homogeneous fluid is known to settle in an oscillatory regime past a critical Ar number ($Ar \approx 120$) [41]. In the cases studied here, only moderate stratification ($Fr = 8$) is considered when increasing Ar . When $Ar = 52$ and $Ar = 105$, no reorientation of the oblate particles was found and the particle dynamics are very similar to the results presented by Ardekani et al. [41] in a homogeneous fluid, with the difference of the flow field as a result of the stratification (entrainment).

For a prolate particle pair ($\mathcal{AR} = 3$), when increasing Ar to 19, a different interaction regime between the prolate particle pair is found. Initially, as the particles accelerate, the trailing particle drafts into the wake of the leading particle. After the drafting phase, the particles come in contact, and the leading particle then tumbles in the y -direction. Further increasing Ar leads to a similar settling regime found when $Ar = 19$. The particles experience a drafting-kissing-tumbling phenomenon, with a decreased drafting phase duration with increasing Ar . Similar to the findings of More et al. [35], the prolate particles do not attain a perfect edgewise orientation when settling in a stratified fluid, which is a key difference to oblate particles.

The results presented here show that the pairwise interaction between a spheroidal particle pair settling in a stratified fluid significantly depends on the particle shape and inertia. For an oblate particle pair, two different regimes were found when increasing Ar , such that the particles experience a drafting-kissing-reorientation regime or a drafting-kissing-settling regime. For a prolate particle pair, a drafting-kissing-tumbling (DKT) regime is found when increasing Ar in this work. The results are comparable to the findings of Ardekani et al. [41] in a homogeneous fluid, as only a moderate Fr is considered. Smaller Fr was considered in the work of More et al. [35] for isolated spheroidal particles in a linearly stratified fluid at large Ar (defined as Ga in their work), where the dynamics are in agreement with the findings found for isolated impervious discs in Chapter 4.

5.4 Increasing N_p for spheres

In this section, we increase the particle number to form a dilute cluster of spherical particles, and we compare our results with existing studies of particle-cluster dynamics in homogeneous (unstratified) fluids. Many studies characterise cluster dynamics using the particle volume fraction in a triply periodic domain (as done by Uhlmann and Doychev [175] for example). In a linearly density-stratified fluid, Doostmohammadi and Ardekani [49] considered a suspension of rigid spheres and used a formulation in which the particle density varies with the local stratifying scalar (via a prescribed particulate thermal expansion coefficient). This choice was made so that, after an initial transient, the particles

Table 5.1: Simulation setup utilised for setups S1 and S2.

Setup	Domain size ($L_x \times L_y \times L_z$)	Mesh size	D_p (mm)	Ar	N_p	$\rho_p/\rho_{f,0}$
S1	$24D_p \times 24D_p \times 96D_p$	$512 \times 512 \times 2048$	0.5	13.1	[3 – 26]	1.141
S2	$12D_p \times 12D_p \times 36D_p$	$384 \times 384 \times 1152$	[0.5 – 2]	[13.1 – 105.2]	10	1.141

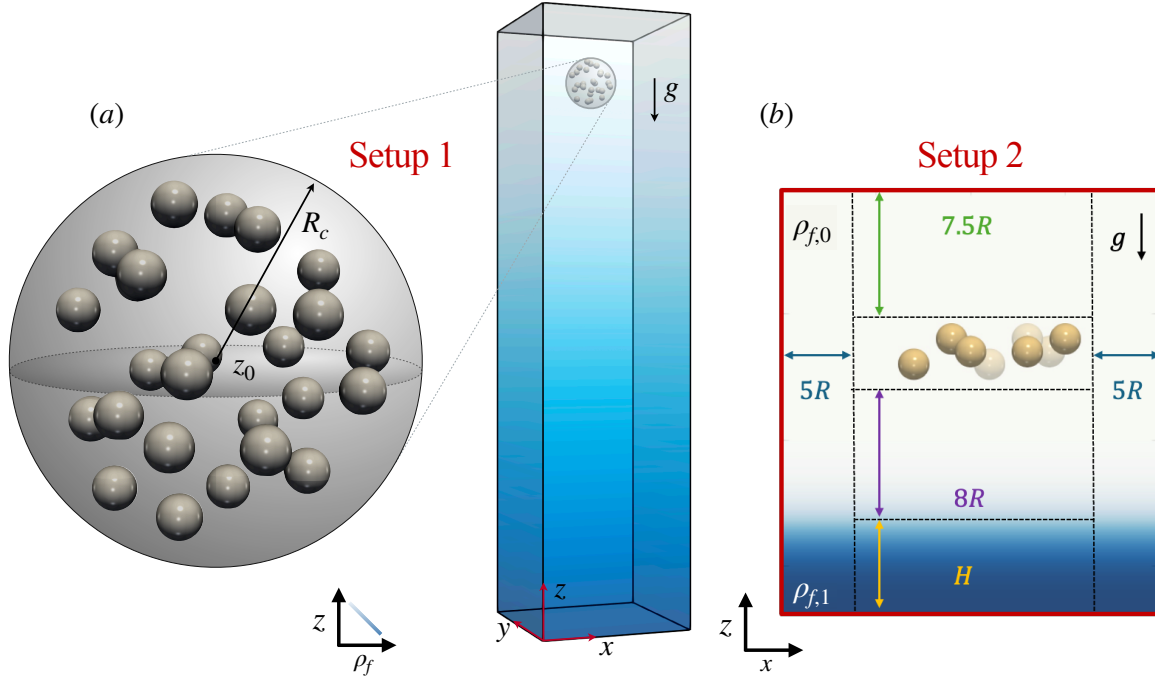


Figure 5.17: Numerical setups used for the simulations of a sparse cluster of spheres with the relevant definitions. Setup 1 and Setup 2 are referred to as S1 and S2 in the text, respectively.

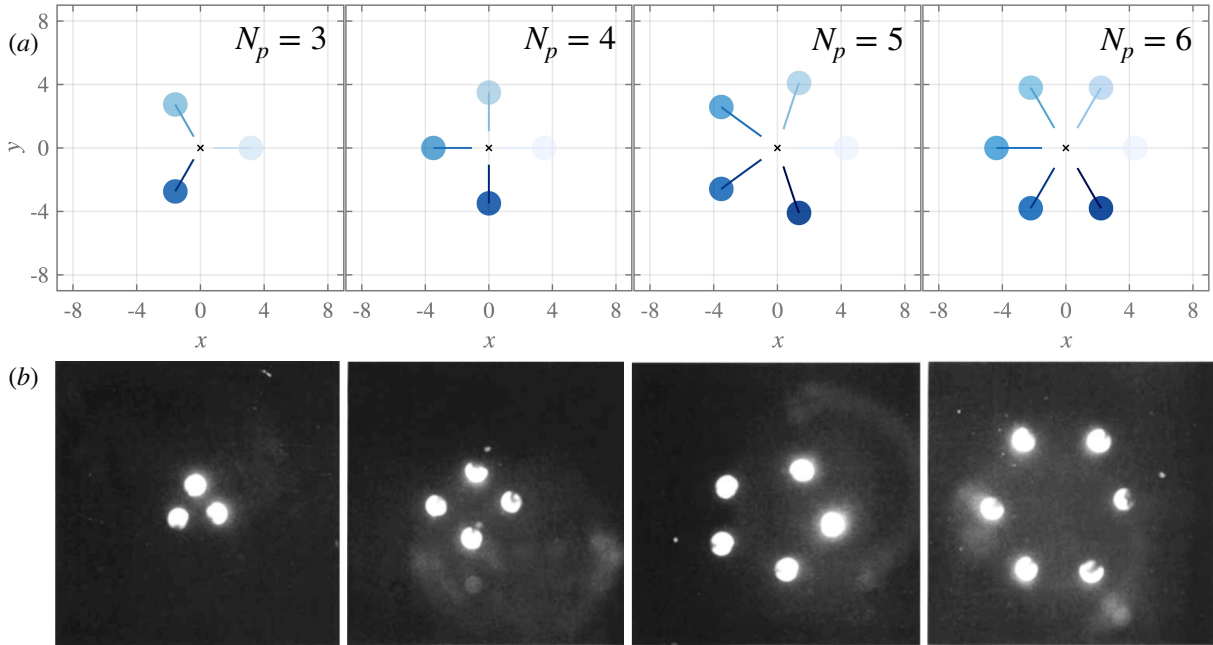


Figure 5.18: Panel (a) shows the top view of the entire simulation using S1 for a sparse cluster of spherical particles with $3 \leq N_p \leq 6$, initialised at the apices of a regular polygon. In panel (b), a top view of the experimental observations of Jayaweera et al. [174] are presented for similar configurations.

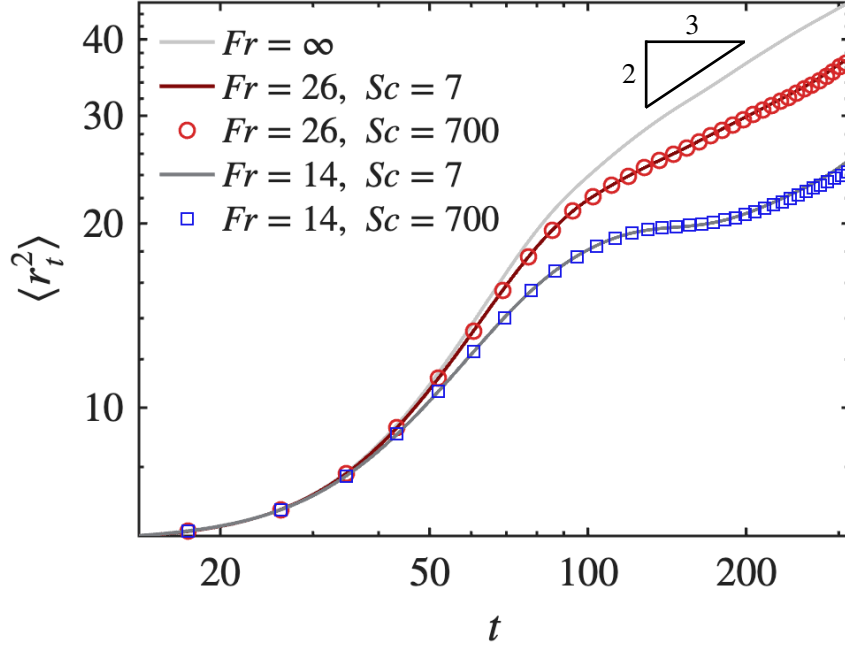


Figure 5.19: Transverse cluster variance $\langle r_t^2 \rangle$ from the simulations using S1 for $N_p = 26$, shown as a log-log plot for varying (Fr, Sc) . After an initial quadratic growth, the homogeneous case exhibits a $t^{2/3}$ scaling, consistent with Subramanian and Koch [53].

approach a steady (or quasi-steady) settling regime rather than continually evolving as they move through the background stratification. As discussed in Chapter 2 for homogeneous fluids, the dynamics of particle suspensions and particle clouds span both viscous and inertial regimes (see for instance the recent review of Fardin et al. [51]). In the Stokes limit, a sedimenting particle cloud is often described by a drop-like behaviour with an internal toroidal recirculation; particles are progressively lost from the rear, producing a trailing tail and eventual cloud disintegration [43, 52]. The cloud stability depends on the particle number N_p , with larger N_p promoting deformation into a torus and subsequent ‘pinch-off’ into daughter clouds in a cascade [52]. As inertia increases, the onset of macro-scale inertial effects is typically associated with a cloud Reynolds number of order unity, while micro-scale inertial effects arise once particle-scale inertial disturbances extend to the cloud boundary and interact with it; in the low but finite- Re limit, this corresponds to the particle-induced Oseen disturbance extending to, and interacting with, the cloud boundary [53].

However, for small particle numbers, the experiments of Jayaweera et al. [174] on small clusters of spheres settling in a viscous fluid reported several characteristic behaviours. Most notably, for compact clusters with $3 \leq N_p \leq 6$ at $Re \lesssim 7$, the particles tend to organise into the vertices of a regular polygon. This polygon then expands with time, with an expansion rate that decreases as the inter-particle separation increases. For larger

clusters, $N_p \geq 7$, there is no clear tendency to form a regular polygon; instead, the cluster typically breaks up into two or more subgroups.

Two numerical configurations are used to study a sparse cluster of spherical particles, as summarised in table 5.1. Setup 1 (S1), shown in panel (a) of Fig. 5.17, is used for simulations in a linearly stratified fluid. Since simulations in this domain are computationally expensive, only a limited set of cases is presented. Setup 2 (S2), shown in panel (b) of Fig. 5.17, is used for an initially quasi-planar cluster traversing a sharp density interface. For both setups, the domain boundary conditions are laterally periodic, with free slip and no penetration at the top and bottom boundaries. Furthermore, utilising S1, we first consider a small number of spherical particles to draw comparisons with the experiments of Jayaweera et al. [174] for $3 \leq N_p \leq 6$ where the particles are initialised in a planar configuration at the apices of a regular polygon. To enable comparison with Subramanian and Koch [53] and Daniel et al. [44], we initialise the particles in a spherical cloud of radius R_c , as shown in panel (a) of Fig. 5.17. The cloud radius is set to $R_c = 4D_p$, and the initial cloud centroid in the vertical direction (z_0) is located a distance $9.6D_p$ below the top boundary ($z_0 = 0.9L_z$). Particle centres are seeded randomly within the cloud while enforcing a non-overlap constraint. In S2, a similar particle seeding mechanism was implemented, with additional constraints shown in panel (b) of Fig. 5.17 to ensure the particles are laterally close to the centre of the domain, and vertically above the density transition region. Because the particles are seeded randomly, the detailed particle–particle interactions within a given cluster are expected to depend on the initial configuration, especially for $N_p > 3$, where interactions among several particles can exhibit strong sensitivity to their initial positions even at low Reynolds number [176]. The present simulations therefore treat individual trajectories and pairwise interaction histories as dependent on the particular initial particle arrangement, and focus instead on collective cluster measures such as the evolution of the cloud centroid, vertical extent, and transverse variance. The aim is to determine how stratification modifies these collective measures relative to homogeneous cases.

For S1, the non-dimensional parameters are defined similarly to the previous cases presented for the interaction between a particle pair, whereas in S2, we utilise Γ (see Eq. 5.4) to quantify the strength of the density transition layer as done by Deepwell et al. [16]. Lastly, in S2, a hyperbolic tangent formulation, where $z_{\text{int}} = 0.7L_z$, is utilised for the density transition layer that follows:

$$\rho_f(z) = \rho_{f,0} + \frac{\rho_{f,1} - \rho_{f,0}}{2} \left(1 - \tanh\left(\frac{z - z_{\text{int}}}{H}\right) \right). \quad (5.14)$$

As we gradually increase the particle count from a pair to small clusters with $3 \leq N_p \leq 6$ in a homogeneous fluid, Fig. 5.18 compares the resulting top-view organisation. In panel (a), the S1 simulations show that particles seeded on the vertices of a regular polygon preserve a polygonal arrangement while the cluster expands in the transverse plane, with the particle paths indicating an outward drift away from the cluster centre. Panel (b) shows corresponding experimental images of Jayaweera et al. [174] for similar configurations, which display the same tendency for small clusters to form and maintain regular polygonal patterns as they evolve.

As we further increase the particle number to form a sparse cloud, we first performed a set of lower-resolution tests with $N_p = 12$, $N_p = 26$, and $N_p = 48$. Based on these tests, $N_p = 26$ was selected as a compromise: it is large enough to recover the expected variance scaling in a homogeneous fluid while keeping particle–particle collisions sufficiently rare. Fig. 5.19 therefore shows the evolution of the transverse cluster variance for the $N_p = 26$ cloud across homogeneous and stratified cases. Here, the transverse cluster variance is computed about the instantaneous cluster centroid,

$$\langle r_t^2 \rangle = \langle (x - x_{cm})^2 + (y - y_{cm})^2 \rangle, \quad (5.15)$$

where $x_{cm}(t) = \langle x \rangle$ and $y_{cm}(t) = \langle y \rangle$ are the time-dependent centroid coordinates. The quantity $\langle r_t^2 \rangle$ is plotted against time on log–log axes for several (Fr, Sc) , allowing changes in the apparent power-law behaviour to be seen directly. At early times all cases exhibit a rapid growth consistent with an initial quadratic regime, reflecting the strong transient as the randomly seeded cloud adjusts from a spherical arrangement to a quasi-planar arrangement and begins to settle collectively. For the homogeneous reference case ($Fr = \infty$), the subsequent evolution follows an approximate $t^{2/3}$ scaling until the particles reach the bottom boundary, in line with the particle cloud behaviour reported by Subramanian and Koch [53]. Introducing stratification modifies this spreading: the growth of $\langle r_t^2 \rangle$ departs from the homogeneous trend and becomes increasingly subdued as stratification effects become stronger. In particular, reducing the Froude number to $Fr = 14$ leads to a clear suppression of the transverse variance at late times relative to both the homogeneous case ($Fr = \infty$) and the weaker-stratification case ($Fr = 26$). By contrast, for a fixed Fr the curves for $Sc = 7$ and $Sc = 700$ are essentially indistinguishable over the time range shown, indicating that the transverse spreading is only weakly sensitive to Sc in these simulations. Overall, while the early-time transient is similar across all cases, the dominant effect is the reduction of transverse dispersion at later times as stratification strengthens (decreasing Fr), consistent with the earlier particle pair results in the SBS configuration where stratification promoted lateral attraction and suppressed transverse

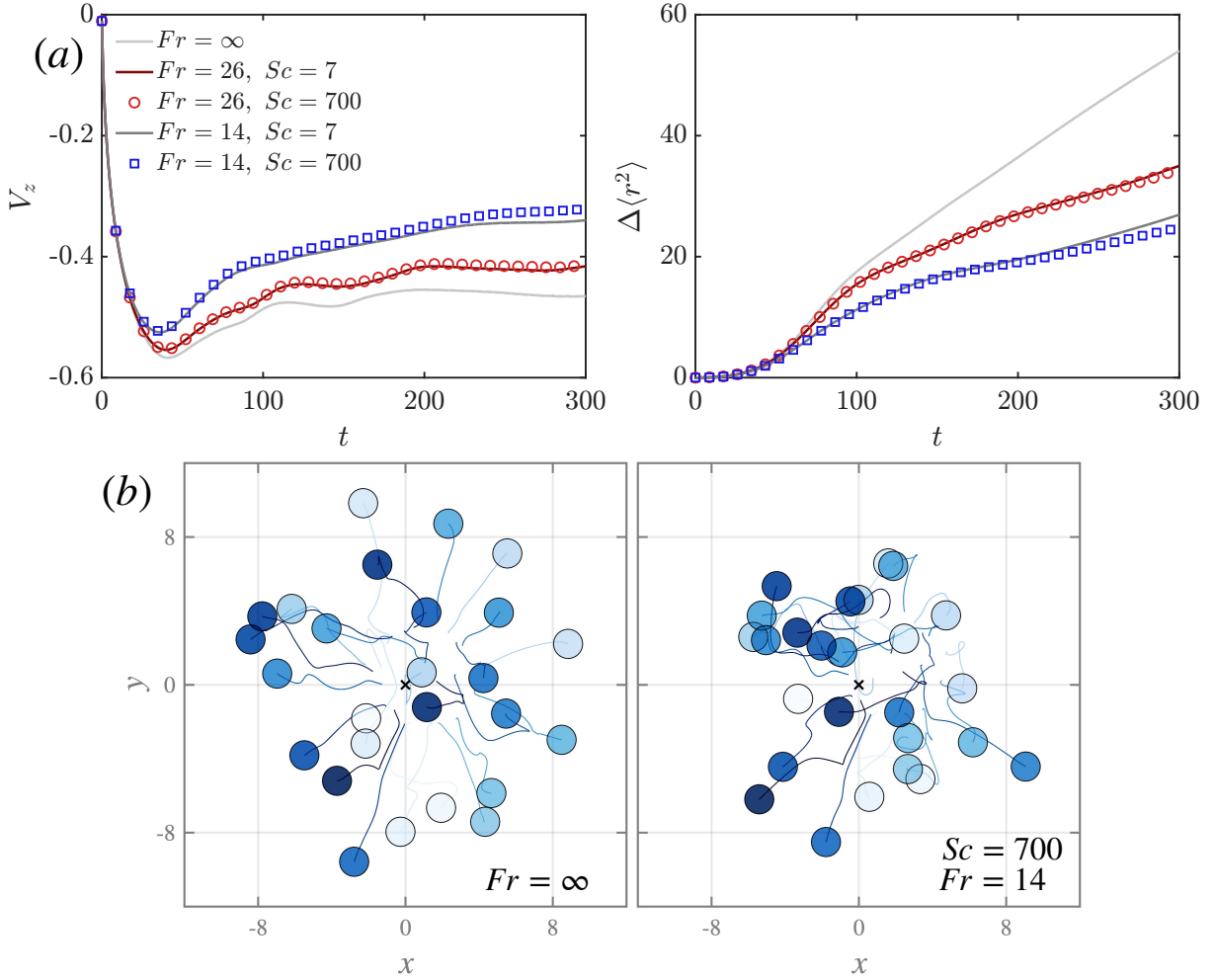


Figure 5.20: Panel (a) shows the settling velocity V_z and the increment of the total mean-square cluster radius $\Delta\langle r^2 \rangle$ (about the instantaneous centroid) for S1 simulations with $N_p = 26$, for varying (Fr, Sc) . Panel (b) shows a top view of the cluster at the end of the simulation for the homogeneous case and for $(Fr, Sc) = (14, 700)$.

separation.

This can be directly seen in panel (b) of Fig. 5.20, where the homogeneous case exhibits a larger lateral dispersion at the end of the simulation, with multiple particles reaching comparatively large transverse distances from the centroid. By contrast, for $(Fr, Sc) = (14, 700)$ the final distribution is more laterally confined, indicating a reduced transverse spread.

The same trend is reflected in panel (a). The settling velocity V_z shows a rapid initial adjustment followed by a slower approach towards an approximately steady value; stronger stratification leads to a reduced settling speed magnitude at late times. In addition, the

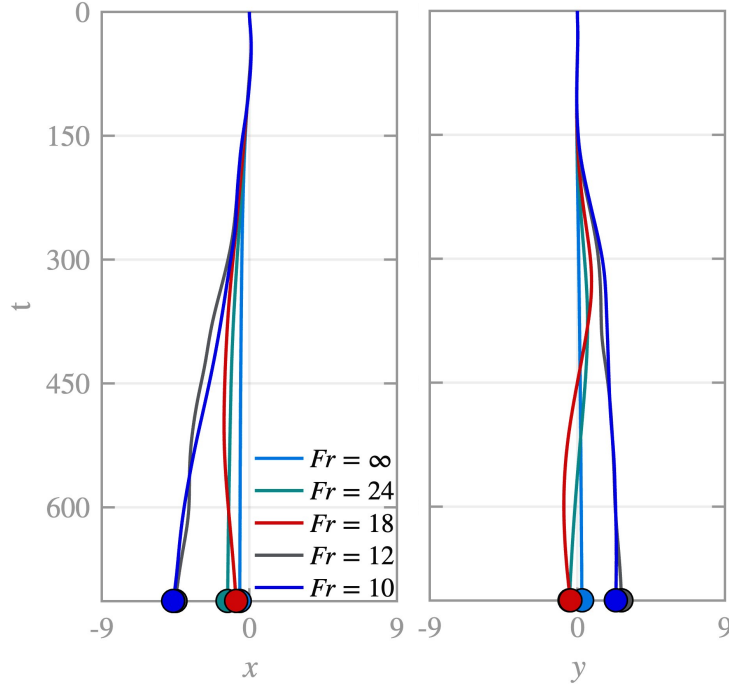


Figure 5.21: Simulations performed using S1 with a resolution of $D_p/\Delta x \approx 16$ for varying Fr and $Sc = 700$ depicting the time history of the centre of mass of the cluster in the x and y directions.

increment of the total mean-square cluster radius,

$$\Delta \langle r^2 \rangle(t) = \langle r^2 \rangle(t) - \langle r^2 \rangle(0), \quad (5.16)$$

with the total mean-square radius about the instantaneous centroid defined by

$$\langle r^2 \rangle(t) = \langle (x - x_{cm})^2 + (y - y_{cm})^2 + (z - z_{cm})^2 \rangle, \quad (5.17)$$

grows more slowly as Fr decreases. This demonstrates that stratification suppresses the overall cloud spreading, consistent with the top-view presentations observed in panel (b).

Preliminary reduced-resolution simulations ($D_p/\Delta x \approx 16$) presented in Fig. 5.21 utilising S1 suggested that, for sufficiently small Fr , the cluster centre of mass can develop a sustained lateral drift, moving away from its initial horizontal position as it settles. Although this behaviour is not examined systematically here, it is qualitatively consistent with experimental observations for falling discs in linearly stratified fluids reported by Lam et al. [40], where a net horizontal migration is observed even as stratification reduces the amplitude of side-to-side fluttering. This suggests that strong stratification may generate

a weak but persistent transverse force, such that a reduction in oscillation amplitude for settling discs does not necessarily imply vanishing mean lateral motion, even below the orientation instability threshold. A more complete assessment under the given setup would require targeted simulations at higher resolution and longer integration times to distinguish transient meandering from a robust, stratification driven drift.

Furthermore, Setup 2 (S2) is utilised to isolate the interaction of a sparse, quasi-planar cluster with a sharp density interface. All cases reported here use $N_p = 10$, so that the interface-crossing dynamics can be compared systematically while varying one control parameter at a time. Fig. 5.22 summarises the response of the cluster as it traverses the interface, shown as a function of the vertical distance travelled relative to the initial cluster position, $\Delta z = z_0 - z$. The three columns report the mean settling velocity V_z , the mean lateral speed $V_l = \sqrt{V_x^2 + V_y^2}$, and the transverse variance $\langle r_t^2 \rangle$. The dashed vertical line marks the interface location z_{int} , while the adjacent dotted lines indicate the thickness of the density transition layer, defined here as the interval over which the background fluid density undergoes 95% of its total change. Across all cases, the same qualitative sequence is observed: as the cluster enters the transition layer, V_z undergoes a rapid reduction in magnitude (a strong deceleration), followed by a partial recovery after crossing; concurrently, V_l exhibits a localised peak within the transition region, with weaker oscillations downstream. The transverse variance typically shows a kink or short plateau near the interface before resuming its downstream growth.

Row (a) varies the stratification strength Γ at fixed $Sc = 7$ and $Ar = 13.1$. Increasing Γ produces a sharper reduction in the magnitude of V_z as the cluster enters the transition layer, and delays the subsequent recovery, indicating a stronger and more persistent deceleration. Consistently, the lateral particle speed V_l is increasingly reduced when Γ increases as the particles cross the density transition. The transverse variance $\langle r_t^2 \rangle$ exhibits a non-monotonic response: it decreases as the cluster traverses the transition layer, indicating a transient lateral contraction (particle attraction), and then increases again after the cluster exits the transition as the entrained fluid returns towards its equilibrium level. For larger Γ , this contraction phase persists over a wider interval in Δz , consistent with an increased residence time of the cluster within the transition layer.

Row (b) varies the Schmidt number at fixed $\Gamma = 0.6$ (and $Ar = 13.1$). Increasing Sc sharpens the reduction in the settling speed magnitude as the particles traverse the transition layer. This is consistent with reduced scalar diffusion at larger Sc , which allows more light fluid to be entrained and retained around the cluster during the crossing, thereby increasing the effective local stratification experienced by the particles. The correspond-

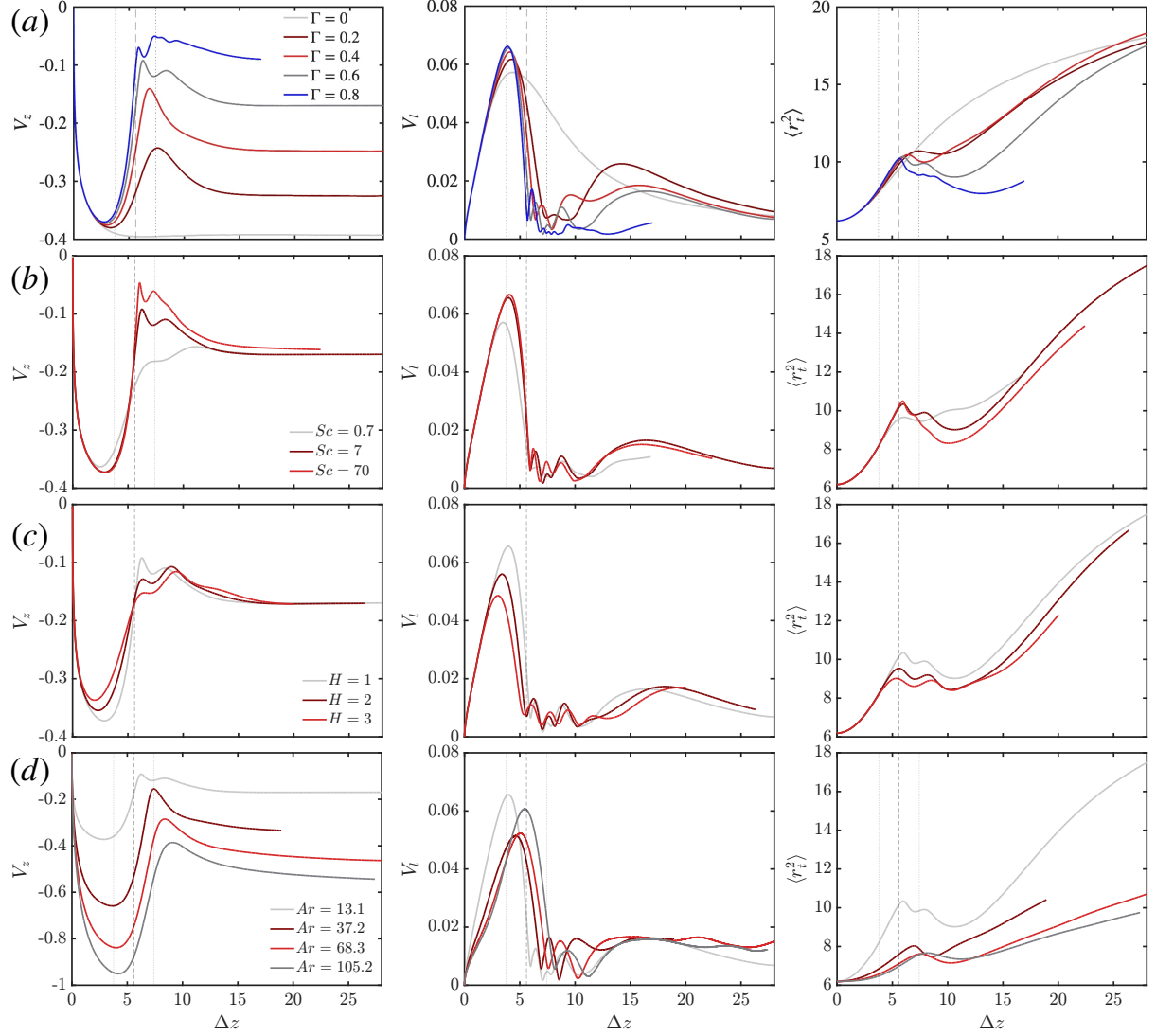


Figure 5.22: Setup 2 (S2): quasi-planar cluster crossing a sharp density transition layer. The dashed line marks the interface position z_{int} , and the dotted lines denote the 95% transition thickness of the prescribed density profile. From left to right, the panels show the mean settling velocity V_z , the mean lateral speed V_l , and the transverse cluster variance $\langle r_t^2 \rangle$, plotted against $\Delta z = z_0 - z$ for $N_p = 10$. Row (a) varies the interface strength Γ (fixed $Sc = 7$, $Ar = 13.1$); row (b) varies Sc (fixed $\Gamma = 0.6$); row (c) varies the transition-layer thickness parameter H ; row (d) varies Ar . Unless otherwise stated, $Ar = 13.1$, $Sc = 7$, $H = 1$.

ing changes in V_l and $\langle r_t^2 \rangle$ are comparatively modest, and the curves approach similar downstream settling values once the entrained light fluid returns towards its equilibrium level.

Row (c) varies the transition-layer thickness parameter H in the density profile. Increasing H spreads the interaction over a wider range of Δz , leading to a smoother crossing. In particular, the peak settling velocity magnitude is smaller for thicker transition layers, but the deceleration is less severe, with V_z varying more gradually through the transition region. The corresponding response in V_l is also weakened: the peak in lateral particle speed observed as the cluster crosses z_{int} decreases in magnitude as H increases. A similar trend is observed for $\langle r_t^2 \rangle$: the transient deviation from its upstream trend during the crossing is weaker for thicker transition layers, while the curves exhibit a similar downstream growth once the cluster has moved below the transition.

Row (d) varies the Archimedes number Ar while holding the remaining parameters fixed. As expected, increasing Ar increases the characteristic settling speed. In these simulations, no particle levitation behaviour is observed (a reversal of V_z), as such behaviour is expected only for thin transition layers [168] and, typically, high Sc (for example $Sc = 700$). The transverse variance shows that the degree to which the transition layer limits lateral spreading depends on inertia, and the stratification-induced reduction of lateral dispersion is less pronounced at higher Ar over the interval shown.

These results provide insight into the dynamics of particle clusters initialised with small inter-particle separations in density-stratified fluids. Stratification is observed to induce an effective attraction between particles, mitigating the lateral spreading that would otherwise occur in a homogeneous fluid. We therefore expect clusters with an initially quasi-planar arrangement to remain more laterally aligned as they settle, with reduced transverse dispersion. However, as N_p increases, this lateral alignment does not necessarily imply that the cluster remains compact in three dimensions. In particular, the quasi-planar configuration can become unstable to vertical rearrangement, leading to the emergence of vertically separated subgroups. Physically, once a few particles (or a small subgroup) move slightly ahead in the vertical direction, they can modify the local flow and scalar field in a way that favours further separation, so that the cloud becomes organised into a leading group and one or more trailing groups rather than a single coherent ‘sheet’, as seen in the simulations of Deepwell and Sutherland [50]. This tendency is expected to be more pronounced for polydisperse suspensions, since larger particles settle faster and can entrain or shelter smaller particles within their wakes, promoting preferential alignment in the vertical direction. Even in the monodisperse case, small particle groups

may transiently behave as a single larger body, generating a stronger wake that can capture trailing particles. Such wake-mediated interactions can therefore promote vertical separation into groups despite the stratification-driven suppression of lateral spreading.

5.5 Concluding remarks

This chapter studies the interaction dynamics between particles in a density-stratified ambient. For a spheroidal particle pair settling in-line in a linearly stratified fluid, the study considers the effects of the stratification strength, characterised by the Froude number (Fr), on the settling dynamics when the Archimedes number $Ar = 4.65$. The particle shape is governed by the aspect ratio $\mathcal{AR} = 1/3$ and $\mathcal{AR} = 3$ for an oblate or prolate spheroid, respectively. The results showcase an initial drafting phase of the trailing particle into the leading particle's wake, followed by a separation phase of the two particles due to the effects of the stratification. During the drafting phase, a buoyant jet forms behind the trailing particle due to the restoration of the pycnoclines to their neutrally buoyant position. As the particles separate, a secondary jet forms in the region between the leading and the trailing particles, which causes the trailing particle to reorient. The reorientation was found to be more significant for the oblate cases when compared to the prolate cases. For the oblate cases, the secondary jet causes the trailing particle to tilt and escape the wake of the leading particle, leading to an asymmetric side escape regime. Increasing the initial separation distance between the two particles led to an earlier onset of the secondary jet between the two particles. Additional aspect ratios were considered for the oblate cases, such that $\mathcal{AR} = 2/3$ and $\mathcal{AR} = 1/2$ at large Sc numbers. At these aspect ratios, the trailing particle was still found to escape the wake of the leading particle, with decreased lateral drift with increasing $\mathcal{AR}$. Further simulations exploring smaller Sc showed that the strength of the transient jet in the gap region between the particle pair decreases, such that no reorientation of the trailing particle was observed in the present simulations. The role of Ar at moderate Fr and Sc showed that the dynamics follow closely the results of Ardekani et al. [41] in a homogeneous fluid, where different settling regimes are observed compared to $Ar = 4.65$.

When increasing N_p , the sparse cluster simulations of spherical particles show that stable density stratification fundamentally alters particle–particle interactions and the resulting cloud evolution. For clusters initialised with small separations, stratification promotes an effective lateral attraction that suppresses transverse spreading relative to the homogeneous case, leading to more laterally aligned configurations as the particles settle.

For larger clouds (for example $N_p = 26$), this manifests as a clear reduction in the growth of the transverse cluster variance at late times as Fr decreases. In the sharp-transition configuration (S2, $N_p = 10$), the crossing is characterised by a strong reduction in $|V_z|$ through the transition layer together with a localised increase in lateral particle motion; importantly, the transverse variance can decrease during the crossing (transient contraction) before increasing again once the entrained light fluid returns to its equilibrium level below the transition. Parameter variations indicate that stronger stratification (larger Γ) and weaker scalar diffusion (larger Sc) intensify the slowdown by increasing the effective local stratification experienced by the cluster, while a thicker transition layer (larger H) smooths the response. A final observation with potential implications is that, although stratification tends to maintain lateral coherence, increasing N_p can still favour vertical reorganisation: quasi-planar arrangements may become unstable to vertical separation into leading and trailing subgroups through wake-mediated interactions, and this tendency is expected to be stronger for polydisperse suspensions where settling large particles can entrain and shelter smaller particles in their wakes. Preliminary reduced-resolution cases also suggested that at sufficiently small Fr the cluster centre of mass may drift laterally from its initial position, consistent with reported horizontal migration of non-spherical bodies in linearly stratified fluids. Taken together, these trends suggest that stratification can simultaneously suppress lateral dispersion while promoting new pathways for vertical structuring and lateral drift, which may be important for interpreting the transport and mixing induced by particle-laden flows in stratified environments.

This work mainly focused on moderate stratification strengths and particle sizes. These parameters typically correspond to the settling behaviours of particles as found in the ocean [15]. The ultimate goal of this work is to gain insight into the interaction dynamics between particles as found in geophysical applications, and future directions could include the study of the collective transport of a large number of non-spherical particles in such stratified environments. Further work investigating the role of the associated induced mixing is warranted for particle clusters traversing a stratified fluid, especially at high Re .

Chapter 6

On the interaction between a settling particle and a deformable interface

Contents

6.1	Introduction	133
6.2	Numerical setup	134
6.2.1	Three-phase contact line	137
6.2.2	Benchmark tests	138
6.3	Results and discussion	141
6.3.1	In-line bubble-particle interactions	141
6.3.2	Off-centre bubble-particle interactions	155
6.4	Concluding remarks	157
6.5	Resolution tests	159

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6.1 Introduction

The transport and dynamics of rigid or deformable particles and their interaction with surfaces are of considerable importance in various scientific and industrial fields due to their potential for efficient, and sustainable applications. Understanding these interactions is crucial for optimising processes ranging from wastewater treatment to mineral beneficiation and food processing. In many engineering applications, a deformable surface, or interface separating two fluids, affects the motion of rigid or deformable bodies. Furthermore, in oceanography, bubbles rising in the ocean may also interact with sedimenting particles, which may play a role in their transport [72].

As suggested in Chapter 2, the dynamic behaviour of bubbles in these processes is crucial. The dynamics of bubbles impacting a solid horizontal wall has been extensively studied in the literature [73–75], where bubble rebound is often found when the bubble approach velocity is sufficiently high. A liquid film that starts to drain in the gap region between the bubble and the solid surface may form when the approach velocity is small. As the deformation of these bodies can be characterised across six orders of magnitude in length scales, there are many difficulties when studying the dynamic nature of the interaction both experimentally and numerically. Numerically, the adhesion behaviour of a bubble to form a three-phase contact line is difficult to predict, since it depends sensitively on interfacial physics that are not resolved by the continuum equations at the grid scale.

In this chapter, we perform DNS to study the dynamic interaction between a rising bubble and a settling particle that are initially released a close distance from one another. Two different interactions are studied, and they are in-line interactions and off-centre interactions. The Archimedes number, defined here as $Ar = \rho_l(\zeta_p g)^{1/2} R^{3/2} / \mu_l$, where $\zeta_p = (\rho_p - \rho_l) / \rho_l$, is utilised for the particle [12]. For the bubble, a Galilei, $Ga = \rho_l g^{1/2} R^{3/2} / \mu_l$, and Bond, $Bo = \rho_l g R^2 / \gamma$, number, where γ is the surface tension, are defined. Herein, the subscripts (l, b, p) denote the background liquid, the bubble, and the solid phase, respectively

The aim of this chapter is to investigate the interaction between a freely rising, deformable bubble and a freely settling spherical particle in a quiescent, Newtonian fluid. This study examines the impact of several parameters on the interaction behavior, including the Galilei number, the Bond number, the density contrast between the solid and the fluid (ζ_p), the ratio of the bubble radius to the particle radius, here defined as Ω , and the surface wettability characteristics of the particle. The outline of the chapter is as follows:

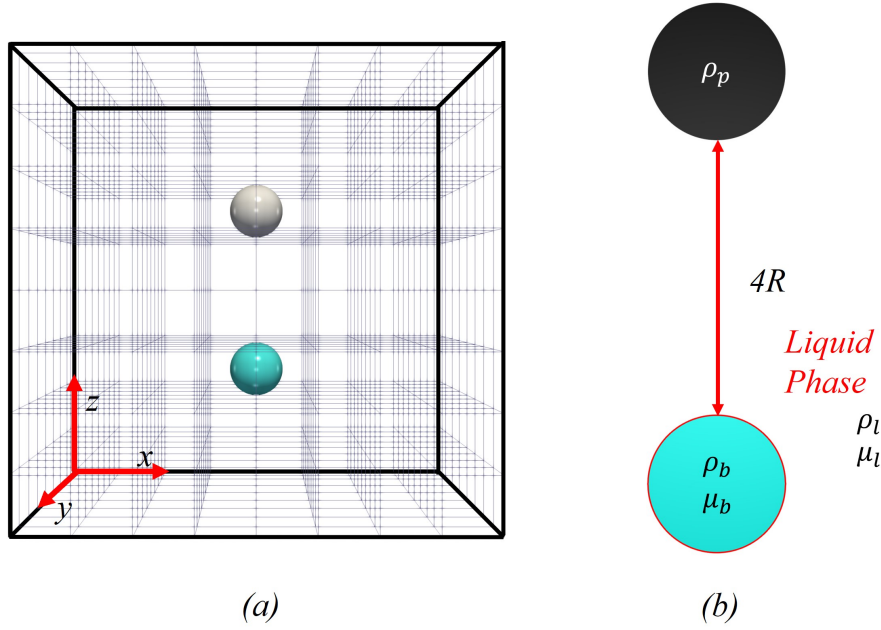


Figure 6.1: (a) The three-dimensional Cartesian cubic domain with a size of $16R \times 16R \times 16R$, showing the subdomain decomposition and the initial problem setup; (b) the initial separation distance between the particle and the bubble is shown.

Section 6.2 contains the numerical setup; Section 6.3 provides a discussion of the results; Section 6.4 contains concluding remarks. Since publication of the manuscript on which this work is based [177], several new studies have examined interactions between bubbles and particles. A brief overview of these developments is included in Section 6.4, together with an outline of directions for future work.

6.2 Numerical setup

This section contains the problem formulation, governing equations, and the numerical setup used in this chapter. We perform highly-resolved numerical simulations of the incompressible Navier-Stokes equations in a three-dimensional cubical Cartesian domain with $L_x = L_y = L_z = 16R$, as shown in Fig. 6.1, where R is the bubble radius. The computational domain is divided into parallel subdomains, which are each uniformly discretised by a 64^3 finite-difference mesh. Within the single-fluid formulation, the material properties in the domain are calculated as follows:

$$\rho(\mathbf{x}, t) = [\rho_b + (\rho_l - \rho_b)\mathcal{H}_f(\mathbf{x}, t)] \mathcal{H}_s(\mathbf{x}, t) + \rho_p(1 - \mathcal{H}_s(\mathbf{x}, t)), \quad (6.1)$$

$$\mu(\mathbf{x}, t) = [\mu_b + (\mu_l - \mu_b)\mathcal{H}_f(\mathbf{x}, t)] \mathcal{H}_s(\mathbf{x}, t) + \mu_p(1 - \mathcal{H}_s(\mathbf{x}, t)), \quad (6.2)$$

A smoothed three-dimensional Heaviside function $\mathcal{H}_f(\mathbf{x}, t)$ for the fluid phases is defined as zero in the bubble phase, and unity in the background liquid phase. A similar approach has been used for defining the properties of the solid particle, $\mathcal{H}_s(\mathbf{x}, t)$ which is considered as zero in the solid phase and unity for both fluid phases (the bubble and the surrounding liquid).

To non-dimensionalise the governing equations, we introduce the following scaling:

$$\begin{aligned} (x, y, z) &= R(\tilde{x}, \tilde{y}, \tilde{z}), \quad \mathbf{u} = \sqrt{gR} \tilde{\mathbf{u}}, \quad t = \left(\frac{R}{\sqrt{gR}} \right) \tilde{t}, \\ p &= (\rho_l g R) \tilde{p}, \quad \mu = \mu_l \tilde{\mu}, \quad \rho = \rho_l \tilde{\rho}, \end{aligned} \quad (6.3)$$

where the tildes, introduced temporarily, designate dimensionless variables. After dropping the tildes, the non-dimensional governing equations read:

$$\nabla \cdot \mathbf{u} = 0, \quad (6.4)$$

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p - \rho \mathbf{e}_z + \frac{1}{Ga} \nabla \cdot [\mu (\nabla \mathbf{u} + \nabla \mathbf{u}^T)] + \frac{\mathbf{F}}{Bo} + \mathbf{F}_{FSI}, \quad (6.5)$$

where $\mathbf{e}_z$ denotes the unit vector in the z -direction (see Fig. 6.1), Ga is the Galilei number and Bo is the Bond number. The non-dimensional material properties then read:

$$\rho(\mathbf{x}, t) = \left[\frac{\rho_b}{\rho_l} + \left(1 - \frac{\rho_b}{\rho_l} \right) \mathcal{H}_f(\mathbf{x}, t) \right] \mathcal{H}_s(\mathbf{x}, t) + \frac{\rho_p}{\rho_l} (1 - \mathcal{H}_s(\mathbf{x}, t)), \quad (6.6)$$

$$\mu(\mathbf{x}, t) = \left[\frac{\mu_b}{\mu_l} + \left(1 - \frac{\mu_b}{\mu_l} \right) \mathcal{H}_f(\mathbf{x}, t) \right] \mathcal{H}_s(\mathbf{x}, t) + \frac{\mu_p}{\mu_l} (1 - \mathcal{H}_s(\mathbf{x}, t)). \quad (6.7)$$

The mesh size used in this study is 512^3 , which corresponds to a resolution of $R/\Delta x = 32$. No-penetration boundary conditions are imposed on the lateral domain walls, and no-slip, no-penetration boundary conditions are imposed on the top and bottom boundaries. The global mesh contains approximately 1.34×10^8 grid points and is decomposed into 512 parallel subdomains. Representative simulations were advanced for $\mathcal{O}(10^4)$ time steps using 512 parallel processes distributed over 8 CPU compute nodes and required approximately seven days of wall-clock time.

In this chapter, the viscosity ratio $\lambda = \mu_l/\mu_b = 100$, and the density ratio $\beta = \rho_l/\rho_b = 1000$ between the bubble and the background fluid are kept constant. The bubble and the particle radii are kept constant $\Omega = R_b/R_p = 1$ unless otherwise stated, with an initial distance of $6R$ from the center of the bubble to the center of the particle. Unless otherwise stated, the particle Archimedes number ($Ar = 10$) is kept constant by setting $\zeta_p = 1$. This

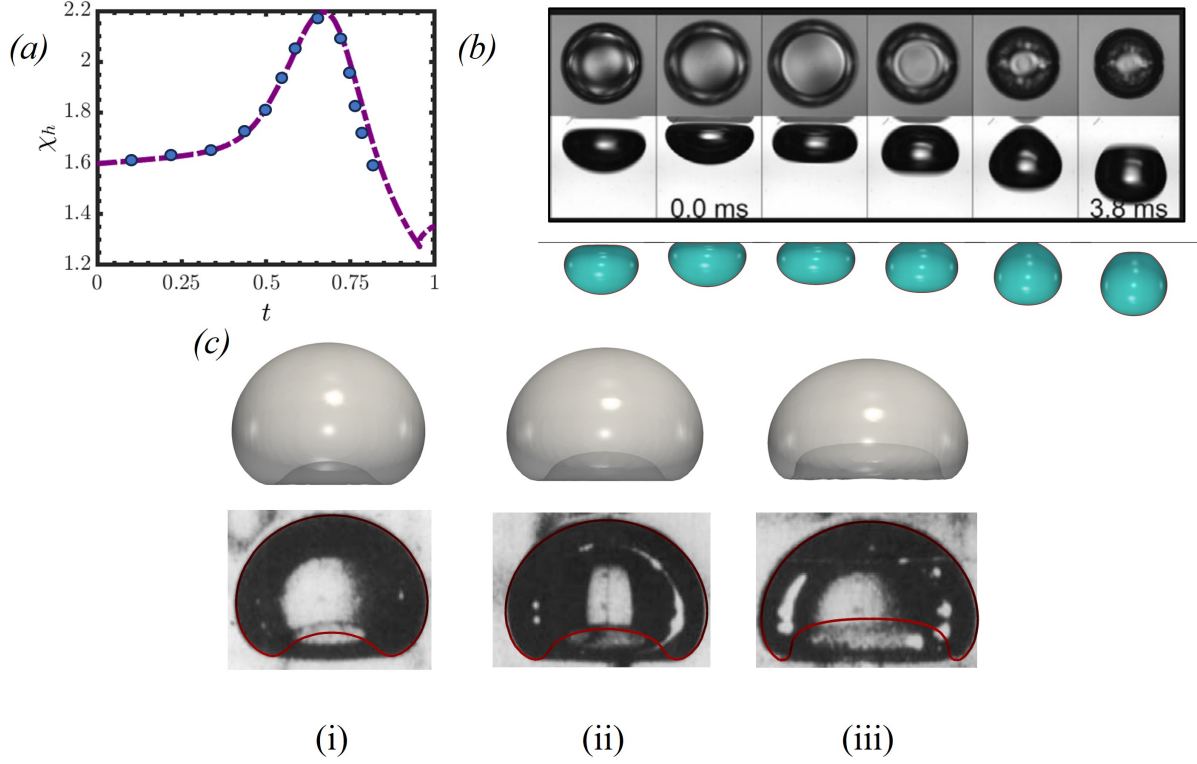


Figure 6.2: Validation of the numerical technique: Panels (a) and (b) show a comparison of our predictions with the experimental data of Kosior et al. [178] for a freely-rising bubble interacting with a solid wall; (a) compares the bubble deformation as a ratio of the horizontal over the vertical bubble axis, and (b) depicts the spatio-temporal evolution of the bubble-wall collision; (c) (i)-(iii) compare the results of a rising bubble shape with the experimental results of Bhaga and Weber [61]. The top panel shows the three-dimensional illustrations of the terminal bubble shapes, and the bottom panel illustrates a slice of the interface superposed on the experimental results of Bhaga and Weber [61]. The parameter values are $(Ga, Bo) = (2.316, 29)$, $(3.094, 29)$, and $(4.935, 29)$ for panels (i), (ii), and (iii), respectively.

study explores the bubble parameter range of $Bo = [0.5 - 5]$ and $Ga = [10, 20]$; Ga is kept relatively low to explore the regime wherein the bubble follows a rectilinear path and interacts with the settling particle.

6.2.1 Three-phase contact line

To mitigate the stress singularity at the contact line [179], the Generalised Navier Boundary Condition is employed in the framework of the LCRM to model the contact line motion [124, 180], which may be crucial for the interaction between bubbles and particles over a certain range of parameters as will be discussed in the following section. Derived from molecular dynamics simulations [181], the boundary condition indicates that the interaction force in a thin layer adjacent to the solid wall includes contributions from both viscous shear stress and an uncompensated Young's stress. The boundary condition thereby combines Navier slip, which relates the contact line displacement to the shear stress at the wall, with the uncompensated Young's stress. In the present LCRM framework, the contact line is defined as the location where the tracked fluid–fluid interface intersects the solid boundary. This position is obtained from the Lagrangian interface elements adjacent to the wall. The local tangent to this interface element is used to evaluate the apparent contact angle, while an extended interface is constructed near the wall to impose the prescribed contact-angle condition. The resulting uncompensated Young stress is then introduced as a regularised capillary forcing term on the Eulerian grid, so that the contact-line motion is updated implicitly through the momentum equation. This approach models microscale slip information at the macroscale, addressing the infinite shear stress problem near the contact line observed under no-slip conditions. The non-dimensional slip velocity u_{cl} is defined as follows:

$$u_{cl} = \lambda_s \left(\left. \frac{\partial u}{\partial n} \right|_{wall} + \frac{\cos \theta_{\text{ext}} - \cos \theta_{\text{cont}}}{Ca \Delta x} \right), \quad (6.8)$$

where λ_s is the slip length, set at a quarter of the size of a grid cell in this work, Ca is the Capillary number defined as $Ca = \mu_l \sqrt{gR} / \gamma$, θ_{cont} is the apparent contact angle governed by the tangential component of the interface element $\mathbf{t}_{\text{cont}}$, and θ_{ext} is the extended contact angle (see Fig. 6.4) for an extended interface inside the wall modeled by tracing a new vector $\mathbf{t}_{\text{ext}}$ in the extended surface. The extended interface contact angle θ_{ext} is used to

account for the contact angle hysteresis, such that the hysteresis model is as follows:

$$\theta_{\text{ext}} = \begin{cases} \theta_{\text{ext}} = \theta_A & \text{if } \theta_{\text{cont}} > \theta_A, \\ \theta_{\text{ext}} = \theta_R & \text{if } \theta_{\text{cont}} < \theta_R, \\ \theta_R < \theta_{\text{ext}} < \theta_A & \text{otherwise,} \end{cases} \quad (6.9)$$

where θ_A and θ_R are the advancing and receding contact angles, respectively. A limitation of the present numerical framework is that a contact line is assumed to form once the separation between the deformable interface and the solid surface reaches one grid spacing. A similar criterion has also been used recently by Zeng et al. [120] and Zeng et al. [119] in simulations based on a front-tracking framework. Two natural extensions for future work are: (i) implementing adaptive mesh refinement to increase resolution in the vicinity of the interface and near contact region, which would reduce grid dependence in the onset of contact line formation; and (ii) introducing a dedicated subgrid drainage (thin-film) model, for example by prescribing a film thickness evolution law and an associated lubrication based closure, to decouple the near contact drainage dynamics from the grid scale. These improvements are left for future extensions of the present study.

6.2.2 Benchmark tests

The numerical method utilised in this study has been extensively validated with experimental works found in the literature. In Fig. 6.2, two different validation results are provided. Panels (a) and (b) show a bubble rising from rest in a quiescent Newtonian fluid, approaching a terminal velocity, and interacting with a solid, immobile, and impermeable wall. The results are compared to the experimental work of Kosior et al. [178]. The bubble terminal velocity found using this numerical method is approximately 350 mm/s, which is in agreement with the terminal velocity found in the experiments (347 mm/s). Panel (a) shows the temporal evolution of the bubble deformation, defined as the ratio of the horizontal to vertical bubble axis, superposed with the experimental results. Panel (b) compares the bubble shapes obtained from the experiments (top) with those predicted by the numerical method (bottom). While the main deformation sequence is captured, some differences are observed between the simulated and experimental bubble shapes, which may be partly attributed to grid resolution. Panel (c) compares the numerical predictions for a rising deformable bubble in a quiescent Newtonian fluid with the experimental results of Bhaga and Weber [61]. The terminal bubble shapes predicted by the simulations show good agreement with the experimental observations. Furthermore,

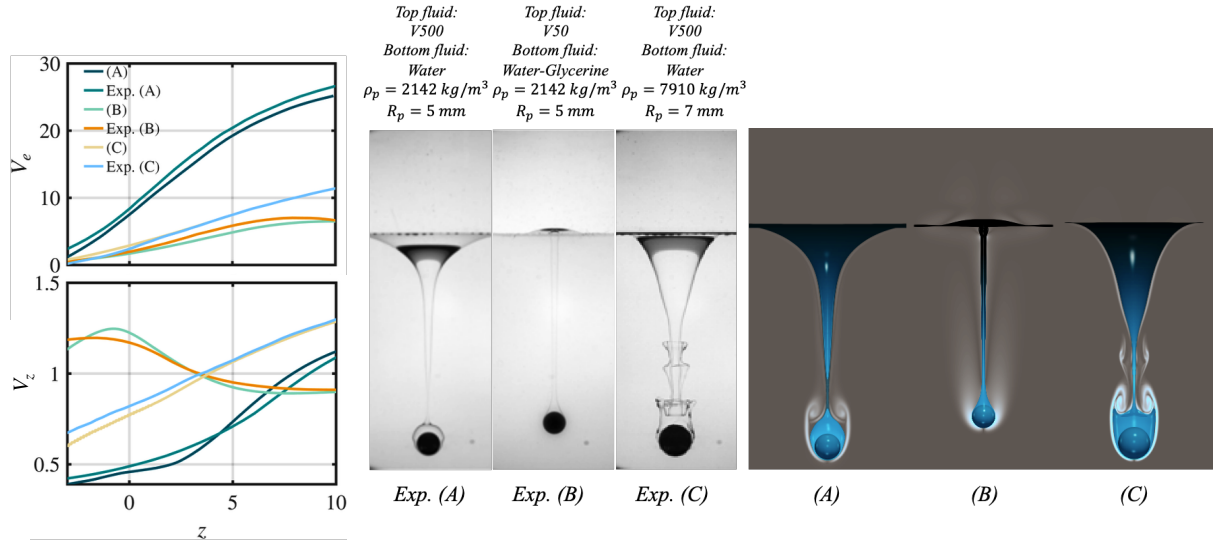


Figure 6.3: This figure showcases the experimental results of Pierson and Magnaudet [102, 103] for a spherical particle crossing an immiscible interface under different configurations. The plots showcase the performance of this numerical method compared to the experimental results in estimating the entrained fluid volume V_e and the particle velocity V_z . Qualitative results from the simulations are also provided.

the numerical framework was validated against experimental measurements for settling solid particles [147, 148], as presented in Chapter 4. We now extend this validation by considering interactions between a particle and a deformable interface.

Additional validation cases are presented for a solid particle settling through an initially unperturbed interface with different fluid and particle properties. The particle was initially placed a distance of $6R$ away from the unperturbed interface (from the centre of the particle) and is allowed to settle due to gravity. The results attained from the numerical method are in close agreement with the results of the experiments of Pierson and Magnaudet [102, 103], where a few differences were found in the case of a top fluid of V500 silicone oil with water as the bottom fluid and a steel sphere. The differences are mainly in the development of axisymmetric corollas near the particle surface as the particle penetrates the bottom fluid. The reason behind the difference may be attributed to the different initial position of the particle in the experiments as this parameter was not exactly specified, or due to the utilised resolution of the case study, which was $\Delta x/R = 1/32$. Nonetheless, the quantitative results of the entrained volume of the first fluid into the second fluid (V_e) is in close agreement with the experimental results, and the particle settling velocity is accurately captured. We note that in this case study, no contact line forms between the solid and the background fluids, such that silicone oil always wets the solid surface at all times, which is in agreement with the results found in

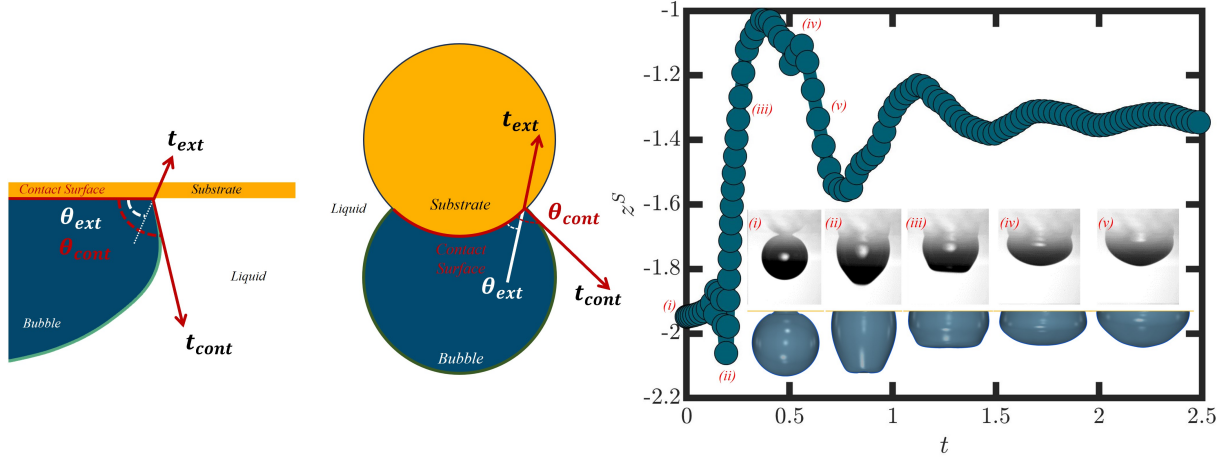


Figure 6.4: The left hand side of the figure provides an illustration of the contact line numerical methodology between a bubble and a solid wall or solid particle. The plot showcases the temporal evolution of the south pole of the bubble as it adheres to a solid wall with negligible inertia. The contact angle for this case was $\theta_A = 102, \theta_R = 99$. A qualitative comparison with the experimental results of Basarova et al. [89] is provided at different time steps.

the experiments of [102]. The entrained volume, V_e , is computed from the phase indicator field by integrating the volume of the initially upper fluid that is carried below the initial interface position, while excluding the solid-particle volume. In discrete form,

$$V_e(t) = \sum_{\phi_s(i,j,k) > 0, z_k < z_{int}} [1 - \mathcal{H}_f(i, j, k)] \Delta V_{cell}, \quad (6.10)$$

where z_{int} is the initial interface height, ΔV_{cell} is the Eulerian cell volume, $\phi_s > 0$ denotes cells outside the solid particle, and $1 - \mathcal{H}_f$ gives the local volume fraction of the initially upper fluid.

Furthermore, Fig. 6.4 presents illustrations for the contact line methodology that is utilised in our in-house solver. The adhesion of a bubble on a solid wall is presented and qualitatively compared to the experiments of Basarova et al. [89]. The bubble is initialised close to the flat wall ($0.1R$ from surface to surface), and as the contact line forms, the deformation of the bubble is accurately captured when compared to the results of the experiment. The bubble size is 0.705 mm, and the viscosity and density ratios correspond to an air/water system. The equilibrium contact angle θ_e was set at $\theta_e \approx 100^\circ$, which corresponds to the surface wettability characteristics utilised in the experiments.

6.3 Results and discussion

The purpose of this study is to gain insight into the interaction between a freely-rising deformable bubble and a freely-settling particle. Unless otherwise stated, the particle and bubble radii are kept equal, $\Omega = 1$, and the particle and the bubble are released in-line, with a distance of $6R$ from their relative centres. The results in this section will investigate the effect of the bubble Bond and Galilei numbers on the interaction between a bubble and a particle. This work will also consider the effect of varying the solid-to-fluid density contrast ζ_p , varying the bubble-to-particle size ratio Ω , and the initial bubble position on the interaction dynamics.

6.3.1 In-line bubble-particle interactions

The first part of the discussion will consider the interaction between a rising bubble and a settling particle with $Ar = 10$ ($\zeta_p = 1$) and $Ga = 10$. The bubble Bond number will be varied between 0.5 and 5. At these conditions, the bubble trajectory is expected to follow a rectilinear path as found by Zhang et al. [63]. Since the bubble and the particle are initially released in line, they will interact through head-on collisions. Panels (a) and (b) in Fig. 6.5 show the spatio-temporal evolution of a rising bubble interacting with a settling particle with $Bo = 0.5$ and $Bo = 5$, respectively. As the bubble rises in a quiescent Newtonian fluid, several different bubble-shape regimes were found by Tripathi et al. [60]. Under the conditions considered in this study, the rising bubble has an axisymmetric shape, as seen in panels (a) and (b) of Fig. 6.5.

Prior to the interaction with the settling particle, the bubble is found to rise in a spherical shape when $Bo = 0.5$, and an ellipsoidal shape when $Bo = 5$. This is because when surface tension forces dominate at lower Bo , the deformation of the bubble will be weak [182]. During the initial interaction process, the particle surface begins to deform the bubble as seen in Fig. 6.5 (a) and (b), such that a dimple forms at the bubble apex, the part of the bubble closest to the particle; dimple formation at the bubble apex was observed for all of the parameters studied in the present work, which is expected due to the increase in hydrodynamic pressure in the gap region between the bubble and the particle [79]. The dimple can be characterised by a negative mean curvature in the centre such that $(\kappa_1 + \kappa_2)/2 < 0$, indicating a concave deformation. A liquid film also begins to develop between the bubble and the particle surface, which drains due to capillary and gravitational forces, causing it to thin over time, as seen in Fig. 6.10. The liquid film drainage described in this work during the interaction between the bubble and the

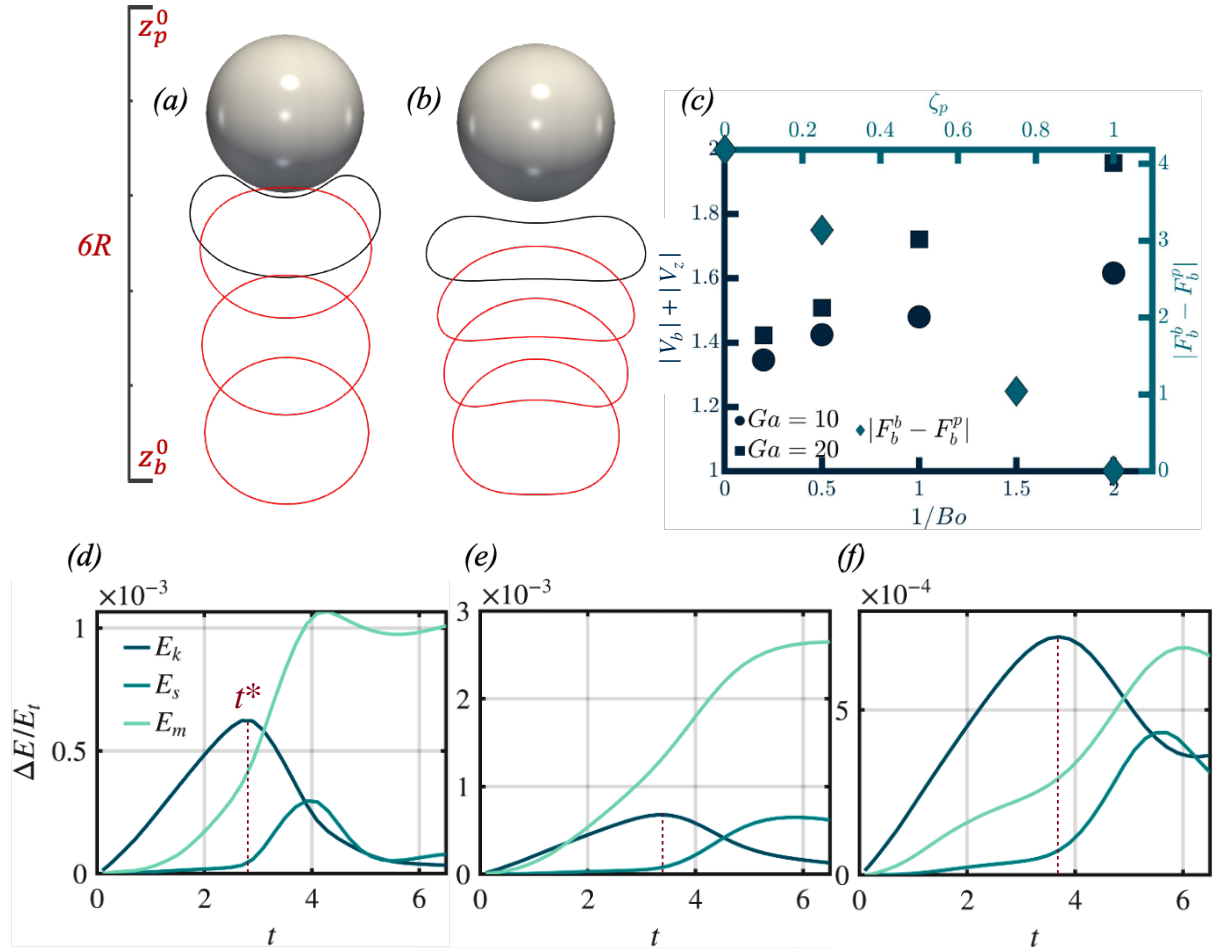


Figure 6.5: Spatio-temporal evolution of the rising bubble as it approaches the particle is shown in (a) and (b). The snapshots of the bubble contours are shown for $t = 1, 2, 3, 4$, and the particle is only shown at $t = 4$. In panel (a), a scale indicating the separation distance is provided between the bubble and the particle, indicating the bubble and the particle's initial centre positions at z_b^0 and z_p^0 , respectively. The non-dimensional parameters are (a) $Bo = 0.5, Ga = 10, Ar = 10$, (b) $Bo = 5, Ga = 10, Ar = 10$; panels (d), (e) and (f) show the change in energy of the system for three different Bo numbers and maintaining $Ga = 10$, and they are $Bo = 0.5, Bo = 2.0$, and $Bo = 5.0$, respectively. Here, E_m is the mechanical energy of the system, such that $\Delta E_m = \Delta E_p + E_k$. A new timescale is introduced here, t^* , which corresponds to the time for the reversal of kinetic energy due to the interaction. Panel (c) showcases the relative velocity of the bubble and the particle when varying Bo and Ga at t^* , and also showcases the difference in buoyancy force between the bubble and the particle when varying ζ_p .

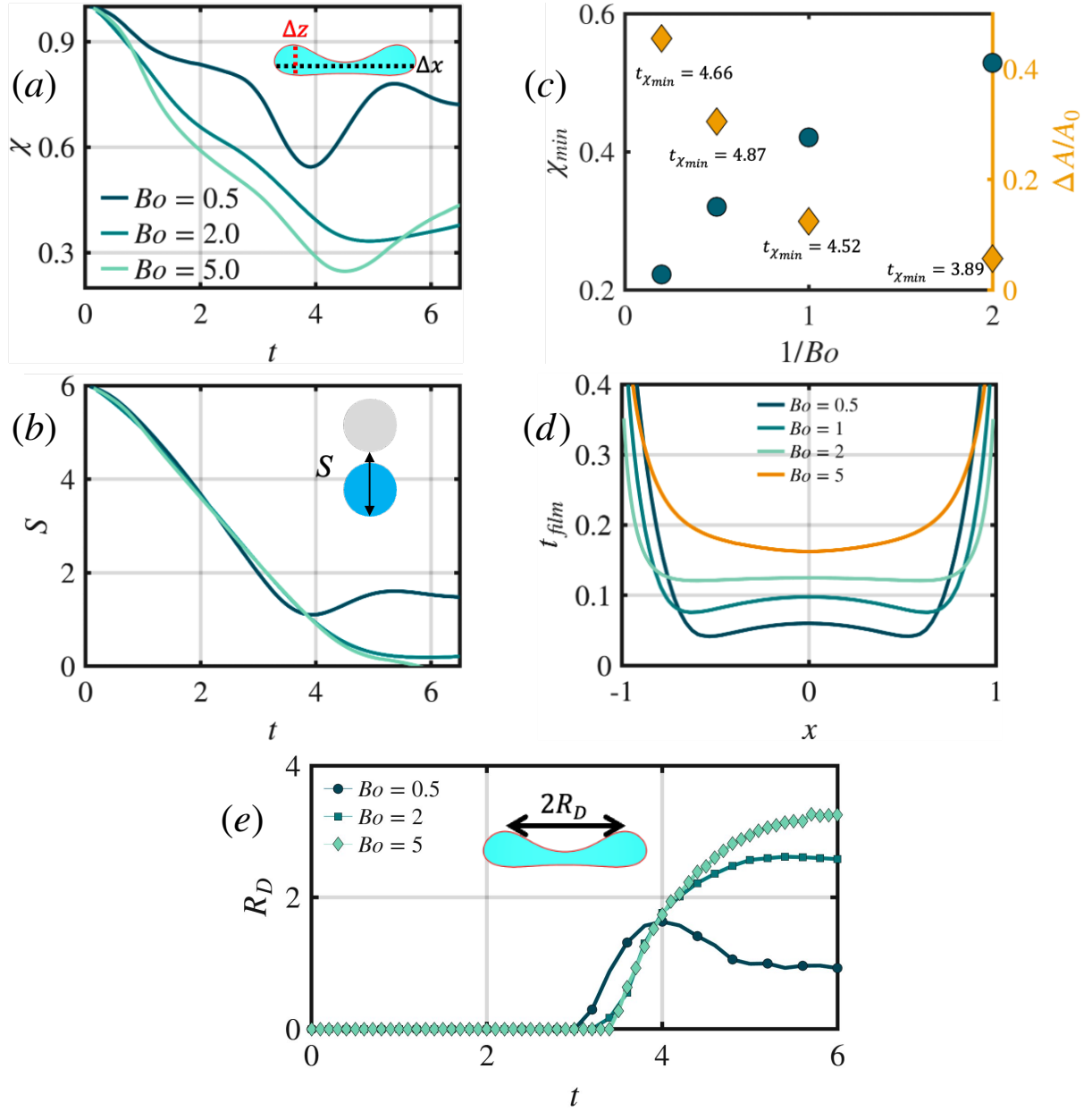


Figure 6.6: Temporal evolution of the aspect ratio, χ , and the distance between the bottoms of the bubble and particle, S , shown in (a) and (b), respectively, for $Bo = 0.5$, $Bo = 2.0$, and $Bo = 5$, with $Ga = 10$, and $\zeta_p = 1$. Panel (c) showcases the minimum aspect ratio when varying Bo and maintaining $Ga = 10$, while also plotting the change in interfacial surface area at that timestep ($t_{\chi min}$). The film thickness profile is presented for these cases at $t_{\chi min}$ in panel (d), and the temporal evolution of the dimple radius R_D is presented in panel (e).

particle, which refers to the thinning of the intervening liquid layer between the bubble interface and the particle surface as the two bodies approach one another, is observed until they are at most one grid cell apart. In dimensional terms, one grid cell is in the order of $\sim O(10\mu m)$, such that the drainage process is purely hydrodynamic and disjoining forces from the interaction can be neglected [183]. Furthermore, the contact line dynamics between the bubble and the particle is considered for different particle wettability parameters.

Upon increasing Bo to $Bo = 2$ or $Bo = 5$, the gravitational forces play a more significant role compared to the surface tension forces. As the bubble and particle approach each other, two distinct observations can be made. Firstly, the onset of dimpling occurs in a position where the bubble and particle are farther away than when $Bo = 0.5$. This can be seen in Fig. 6.5(a,b) and by comparing the bubble aspect ratio χ and the normalised distance S between the bubble and the particle as seen in Fig. 6.6(a,b), respectively; here, χ is defined as the ratio of the bubble's height to its width, and is a measure of its deformation during its rise and interaction with the particle. The dimple formed at the apex is also more pronounced compared to the case when $Bo = 0.5$, and the deformation starts at the cap of the bubble, which leads to a change in the overall bubble shape. The increase in Bond number leads to flattening of the side of the bubble furthest away from the particle, as seen in the interaction between droplets and solid walls at low Reynolds numbers [78]. It proves instructive to carry out an energy analysis of the system when considering the dynamics of the bubble-particle interactions. The four contributions to the total system energy are the potential energy E_p , surface energy E_s , kinetic energy E_k , and viscous dissipation E_η . The changes in the potential and surface energies, respectively, read

$$\Delta E_p = \rho V g(z_c - z_0), \quad (6.11)$$

$$\Delta E_s = \gamma(A - A_0), \quad (6.12)$$

while the kinetic energy and viscous dissipation are expressed, respectively, by

$$E_k = \frac{1}{2}\rho \int_V (u^2 + v^2 + w^2) dV, \quad (6.13)$$

$$E_\eta = \int_0^t \int_V \xi dV dt, \quad (6.14)$$

where A is the bubble surface area, V is the volume of the corresponding phase, z_0 is the bottom of the domain, and $\xi = 2\mu(\mathbf{S} : \mathbf{S})$ is the viscous dissipation function. The temporal evolution of the energy budget during the initial interaction process when $Bo = 0.5$, $Bo = 2$, and $Bo = 5$ are shown in panels (d-f) of Fig. 6.5, respectively. Here,

ΔE_m is the mechanical energy of the system, such that $\Delta E_m = \Delta E_p^{total} + E_k^{total}$, and the results are normalised to the total energy of the system $E_t = E_p + E_k + E_s + E_\eta$. As the bubble rises and the particle settles, E_k is found to increase up to a maximum, until the flow field of the particle and the bubble interact. At this point, E_k starts to decrease as the gap distance between the bubble and the particle thins. We introduce a new time scale t^* which specifies the time of kinetic energy reversal in panels (d-f) of Fig. 6.5. For $Bo = 0.5$, $t^* \approx 3.0$ and for $Bo = 2$ or $Bo = 5$, $t^* \approx 3.5$. In panel (c), the relative interaction velocity at the peak kinetic energy is presented for the case of $Ga = 10$ and $Ga = 20$ when varying the Bo number. When $Ga = 10$, it can be seen that the relative velocity does not vary significantly when increasing Bo , however, the relationship between the relative velocity and Bo remains the same for both Ga . When increasing Bo , the bubble rising velocity decreases, which allows the particle to attain a larger velocity as it settles. However, this increase in particle velocity does not compensate for the difference in bubble rise speed, which causes a decrease in the relative velocity prior to the interaction. A similar trend is observed for $Ga = 20$, with a larger increase in relative velocity when decreasing Bo . Furthermore, the difference in buoyancy force between the bubble and the particle is also presented when varying ζ_p , where the buoyancy force was taken as $F_b^i = Vg(\rho_i - \rho_l)$, where $i = (b, p)$ for the bubble or the particle, respectively. When $\zeta_p = 1$, the buoyancy force of the particle is comparable to that of the bubble, however, decreasing ζ_p leads to a larger difference between the bubble and particle buoyancy force. A larger difference in buoyancy force between the bubble and the particle allows the bubble to ‘push’ the particle upward during the initial interaction, rather than remaining in the same vertical position during film drainage. For low Bo , the particle kinetic energy is seen to decrease to zero at later times, which shows that the film drainage process causes the bubble and the particle to remain at approximately the same vertical position as the liquid film thins (see Fig. 6.5(d)). The formation of the liquid film between the bubble and the particle causes an outward radial velocity of the background fluid, which leads to the dissipation of kinetic energy, as seen at $t = 3.5$ in Fig. 6.7 [81].

As film drainage is a gradual process driven by pressure differences in the film region, this allows time for the surface tension forces to help the bubble recover a semi-spherical shape with a small dimple at the bubble apex. The dimple radius decreases during the drainage of the liquid film, which can be seen at $t \approx 5$ when $Bo = 0.5$ (see Fig. 6.7) and by comparing the liquid film thickness profiles and the bubble interface shape in Fig. 6.8(a,b). Yiantsios and Davis [184] have considered the interaction between a droplet and a solid surface and their numerical simulations showed that the terminal value of the dimple radius scales with Bo as $R_D \sim (\frac{2}{3}Bo)^{\frac{1}{2}}R$, which is in great agreement with the dimple radius found in this work when $Bo = 0.5$ ($R_D \approx 0.5$). This result was first obtained

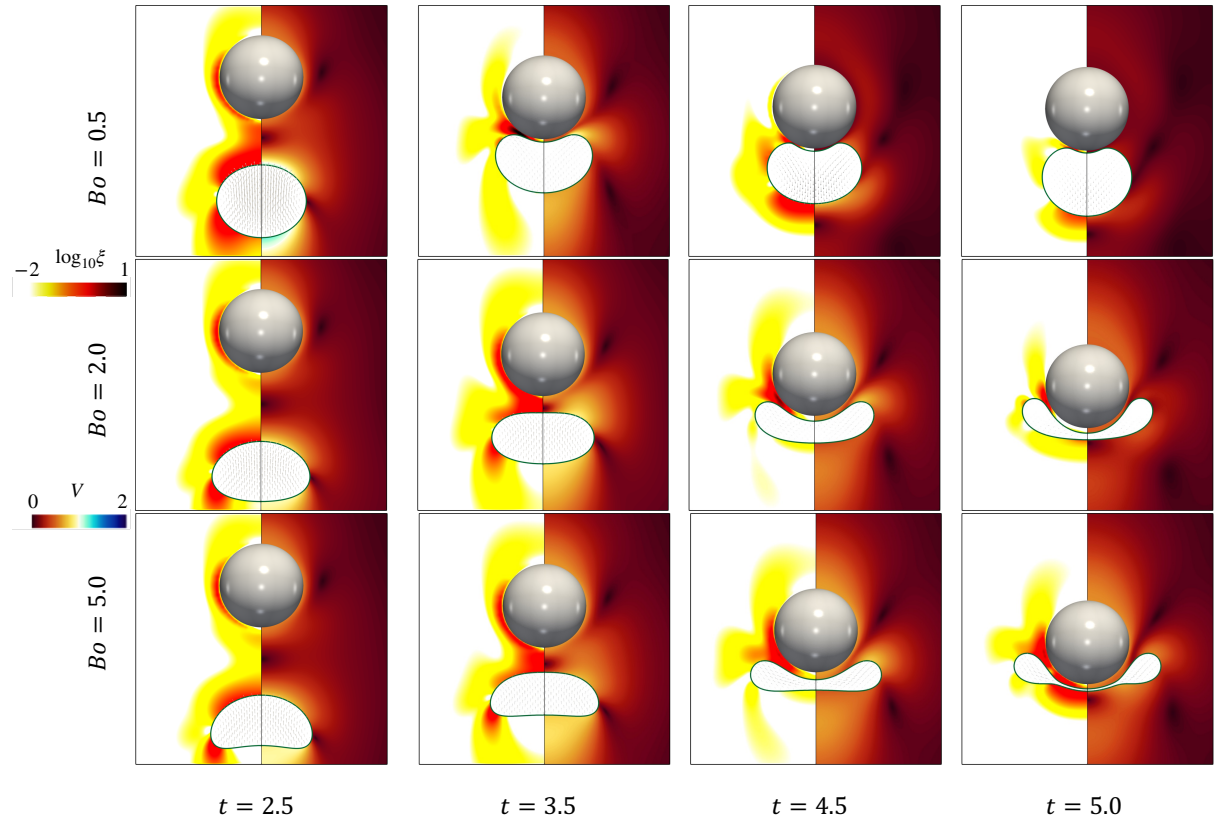


Figure 6.7: Spatio-temporal evolution of the bubble-particle interaction dynamics shown for the same parameters used to generate Fig. 6.5; the rows are associated with $Bo = 0.5$, $Bo = 2.0$, and $Bo = 5$, from top to bottom. The contours on the left part of the figures in the panels show the logarithm of the viscous dissipation function $\log_{10} \xi$ in the fluid, and the contours on the right show the velocity magnitude in the fluid V . The bubble is shown with glyphs of the velocity to illustrate the relative motion of the bubble at different time-steps.

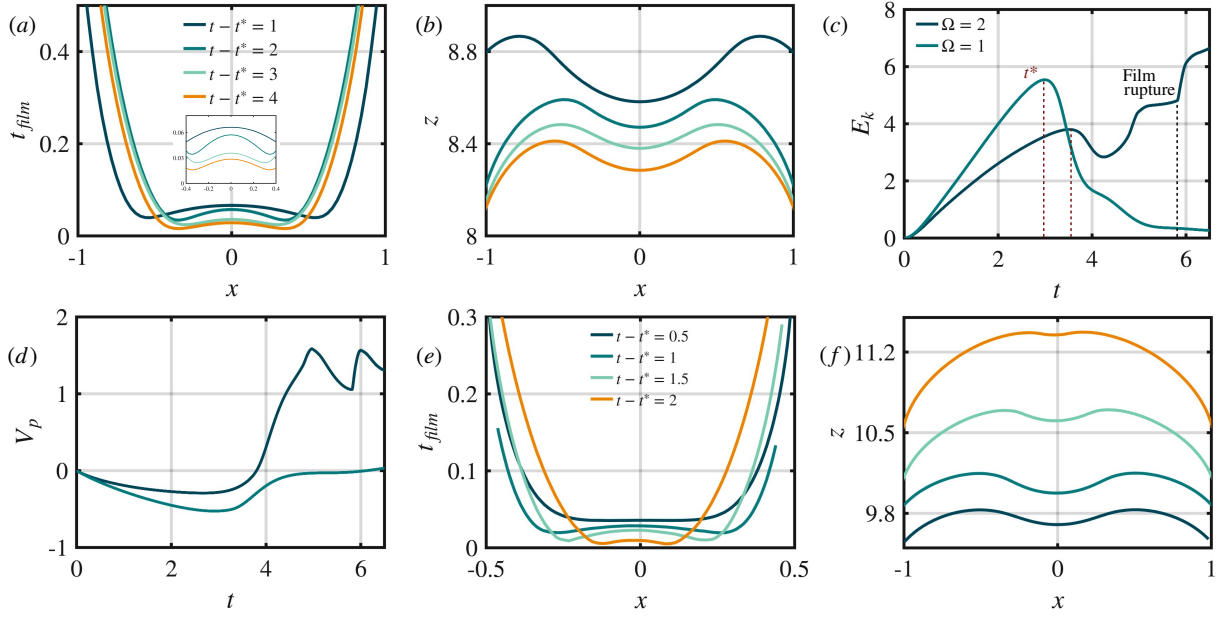


Figure 6.8: This figure showcases the film thickness and the bubble shape as it approaches the particle when $Ga = 10$, $\zeta_p = 1$, and $Bo = 0.5$ in panels (a) and (b). In panels (c) and (d), the temporal evolution of the kinetic energy and particle velocity is presented for two cases, and they are when $\Omega = 1$, which is the base case, and when $\Omega = 2$. In panels (e) and (f), the film thickness profile and the bubble shape at different time steps during the interaction for $\Omega = 2$ are presented.

by Derjaguin and Kussakov [185] by assuming that the pressure in the dispersed phase is approximately equal to the pressure in the dimple and balancing the pressure with the buoyancy force such that $\frac{2\gamma}{R}\pi R_D^2 \sim \frac{4}{3}\pi(\rho_l - \rho_b)gR^3$. In panel (e) of Fig. 6.6, the dimple radius is presented during the initial interaction period for different Bo numbers when $Ga = 10$ and $\zeta_p = 1$, where the scaling of the dimple radius presents a good approximation of the results.

Upon increasing the Bo number to $Bo = 5$, a significantly different interaction process is observed at later times. As the particle deforms the bubble interface, the dimple that forms interacts with the southernmost part of the bubble, such that the bubble will rupture. Prior to its rupture, the bubble is seen to deform severely with a film thickness larger than that associated with the $Bo = 0.5$ case (see panel (d) of Fig. 6.6 and Fig. 6.7 at $t = 5$). The bubble topology resembles the splashing configuration found by Yoon and Shin [186] when considering the interaction between a droplet and a particle, with a liquid film between the bubble and the particle in the present work. In Fig. 6.6, the minimum aspect ratio attained during the interaction is presented when varying Bo in panel (c). The time of maximum bubble deformation (minimum χ) is taken as $t_{\chi_{min}}$, and the change in interfacial surface area $\Delta A/A_0$ is presented. At $t_{\chi_{min}}$, the film thickness profile between

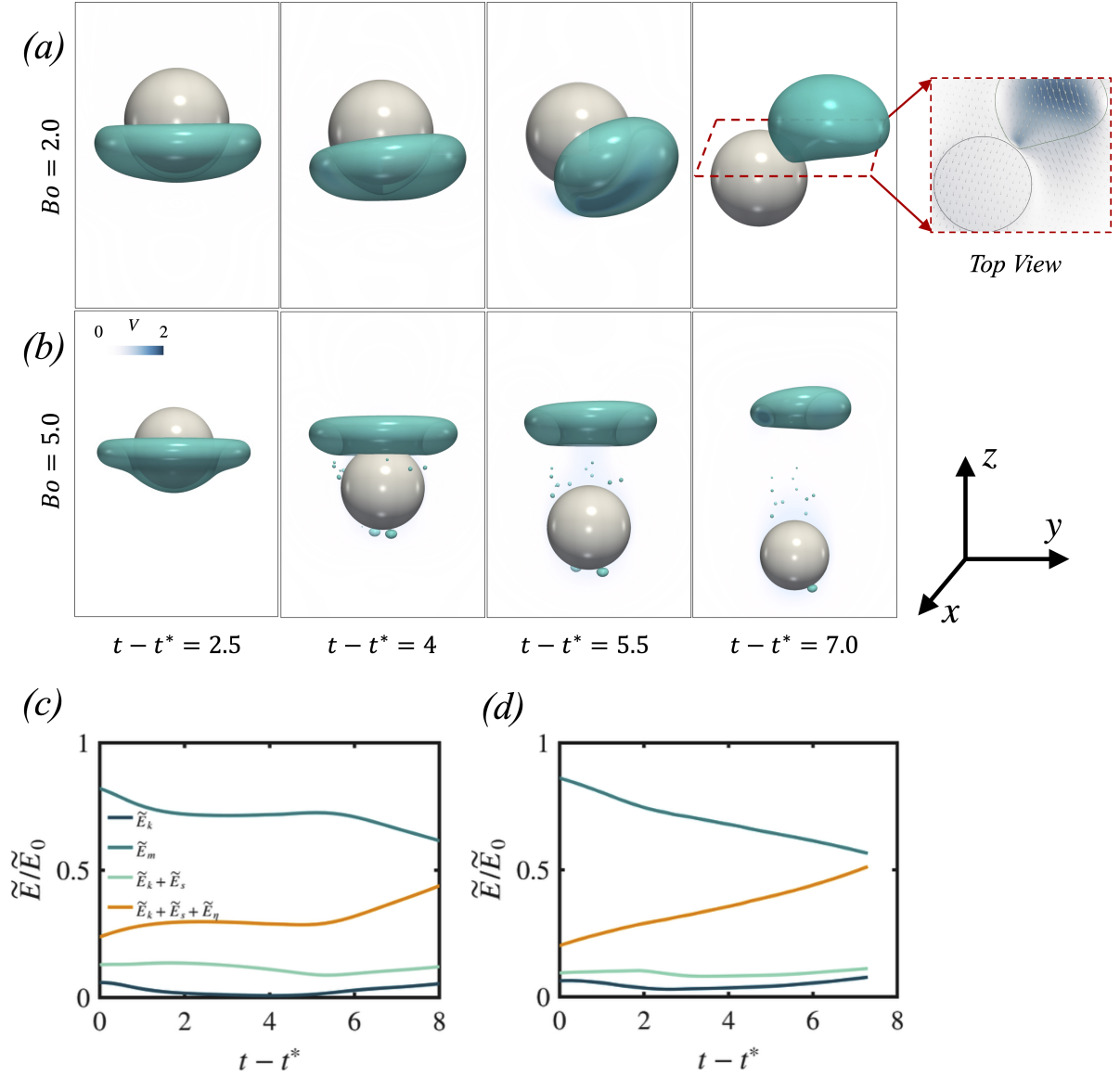


Figure 6.9: The spatio-temporal evolution of the bubble-particle interaction dynamics is shown in (a) for $Ga = 10, Bo = 2$ and $\zeta_p = 1$, where the contours depict the velocity magnitude. Panel (b) shows the spatio-temporal evolution of the interaction dynamics when $Ga = 10, Bo = 5$ and $\zeta_p = 1$. The timesteps presented are relative to t^* , such that $t - t^*$ varies from 2.5 to 7.0. When $Bo = 2$ and $t - t^* = 7$, a top view of the interaction between the bubble and the particle is presented to showcase that no contact is found between them. In panels (c) and (d), the normalised energy budget $\tilde{E}/\tilde{E}_0$ is presented for $Bo = 2$ and $Bo = 5$, respectively, where $\tilde{E}_0 = E_{p_0}^{particle} + E_{s_0}$.

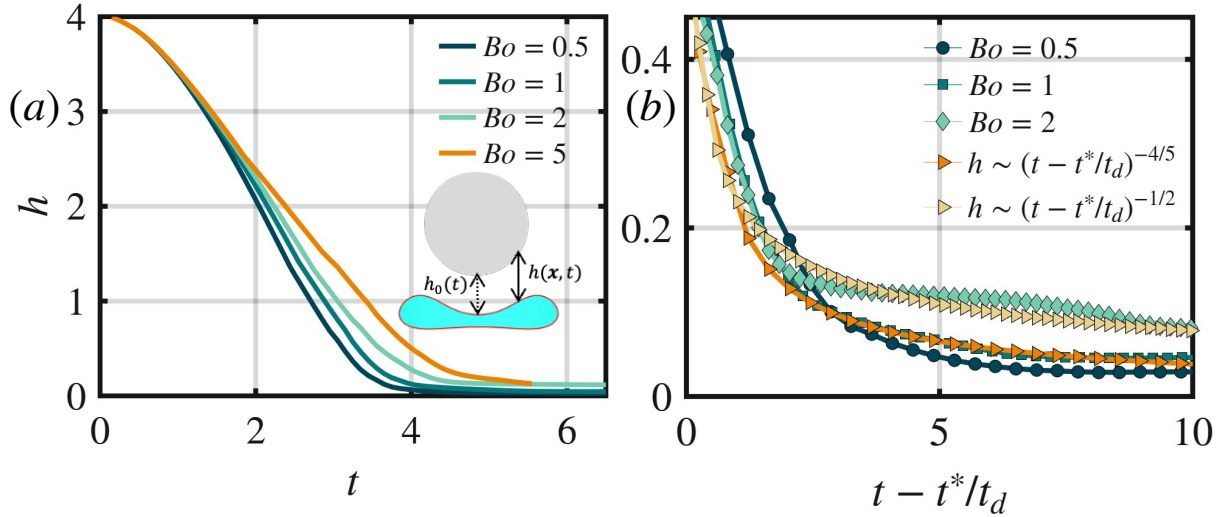


Figure 6.10: Panels (a) and (b) show the temporal evolution of the minimum gap thickness $h(t)$ for different Bo when $Ga = 10$ and $\zeta_p = 1$. Two different scalings are also provided, such that $h \sim (t - t^*/t_d)^{-\alpha}$ where α here is either $4/5$ or $1/2$.

the bubble and the particle is plotted in panel (d). The profiles of the film thickness show that at larger Bo , the minimum gap distance is found at the bubble centre, and when decreasing Bo , the minimum gap distance shifts towards the bubble dimple. The aspect ratio χ reaches a minimum of ~ 0.2 , and the normalised distance between the particle and the bubble, S , continues to decrease. The distortion of the bubble surface caused by the particle drives the increase in χ at later times, up to the point of bubble rupture. Fig. 6.9(b) shows the passage of the particle post-bubble rupture. The particle's kinetic (potential) energy continues to increase (decrease) as seen in Fig. 6.9(d), which shows that the particle continues to settle post-bubble rupture. This bubble rupture mechanism was also found by the two-dimensional, axisymmetric simulations of the interaction between a rising bubble and a solid surface [182], where bubble rupture was observed at large Bo numbers. As the bubble and particle approach each other when $Bo = 2$, the bubble is found to deform similarly to the case $Bo = 5$ (see panel (a) of Fig. 6.6), however, the bubble does not rupture. Therefore, the liquid film in the gap region between the bubble and the particle starts to drain. As the liquid film drains, the buoyancy of the bubble drives it to shift away from the particle, as seen in panel (a) of Fig. 6.9, interrupting the film draining process. As the bubble moves away from the particle, we note that no contact was found between the bubble and the solid surface, as seen from the top view presented. The bubble then continues to rise, and the particle continues to settle, as seen by considering the change in mechanical energy in the energy budget plot presented in panel (c) of Fig. 6.9.

In Fig. 6.10(a, b), the temporal evolution of $h(t)$, defined as the shortest bubble-

particle distance at every time step, is presented for different Bo numbers. As the bubble rises at early times, it assumes a spherical or ellipsoidal shape such that $h(t)$ is measured along centreline of the bubble and particle, which we define as $h_0(t)$. Fig. 6.10(a) provides an illustration of $h_0(t)$ and $h(\mathbf{x}, t)$, such that $h(t) = \min h(\mathbf{x}, t)$. As the dimple forms on the bubble surface, $h(t)$ begins to deviate from $h_0(t)$. When comparing the minimum gap distance for different Bo , it can be seen that for smaller Bo , the film drainage process occurs fastest as the bubble deformations are less severe. This leads to the liquid in the film draining over a smaller surface area [187]. Furthermore, increasing Bo leads to an increase in the surface area in the gap region, which delays the film drainage process. This is found to occur up to $Bo = 2$, because at $Bo = 5$, the bubble ruptures. Comparing the difference between the gap thickness in the centre and the minimum gap thickness when increasing Bo , two different conclusions can be drawn. First, at low Bo , the development of the dimple occurs at earlier times when compared to the larger Bo number cases. However, the dimple is much more pronounced with increasing Bo , at later times. Nevertheless, when the bubble ruptures at $Bo = 5$, the minimum gap distance is always found at the centreline as the particle continues to settle. Previous studies [79, 184, 188–190] have shown that the film thickness during the interaction between a deformable interface and a solid surface scales as $t^{-\alpha}$ where $0 \leq \alpha \leq 1$. During film drainage, we can assume that the outward radial velocity of the fluid is much greater than the vertical velocity of the bubble or the particle. Therefore, a new characteristic velocity scale U can be obtained by balancing the buoyancy and viscous drag ($\Delta\rho R^3 g \sim \mu_l R U$), such that $U = g\rho_l(2R)^2/6\mu_l\phi$ since $\rho_l \gg \rho_b$, and $\phi = (2 + 3/\lambda)/(1 + 1/\lambda)$ is a correction factor for the viscosity ratio λ [190]. We introduce a new draining time scale, $t_d = 2R\sqrt{\mu_l/\gamma U}$, which can be obtained by assuming the film drainage is dominated by the balance of surface tension and viscous stresses [79, 82, 190]. At smaller Bond numbers, the liquid film thickness is found to scale as $h \sim (t - t^*/t_d)^{-4/5}$, whereas when increasing the Bond number, the scale varies to $h \sim (t - t^*/t_d)^{-1/2}$. This result can be seen in panel (b) of Fig. 6.10. We note that when $Bo = 2$, the film drainage result presented is prior to the bubble sliding away from the particle.

Panels (c) to (f) in Fig. 6.8 present the interaction between a bubble and a particle when $\Omega = 2$ when $Ga = 10$, $Bo = 0.5$, and $\zeta_p = 1$. As the bubble and the particle interact, the approach velocity of the particle when $\Omega = 2$ is smaller, such that the larger bubble's kinetic energy is transferred to the particle, allowing it to reverse its direction and float. Here, t^* was found to be around $t \approx 3.5$. As this kinetic energy from the bubble is transferred to the particle, the bubble's second approach to the particle is at a substantially smaller velocity, such that the total kinetic energy stabilises around $t = 5$ to $t = 5.9$. The radius of the dimple on the bubble apex starts to decrease, as seen from

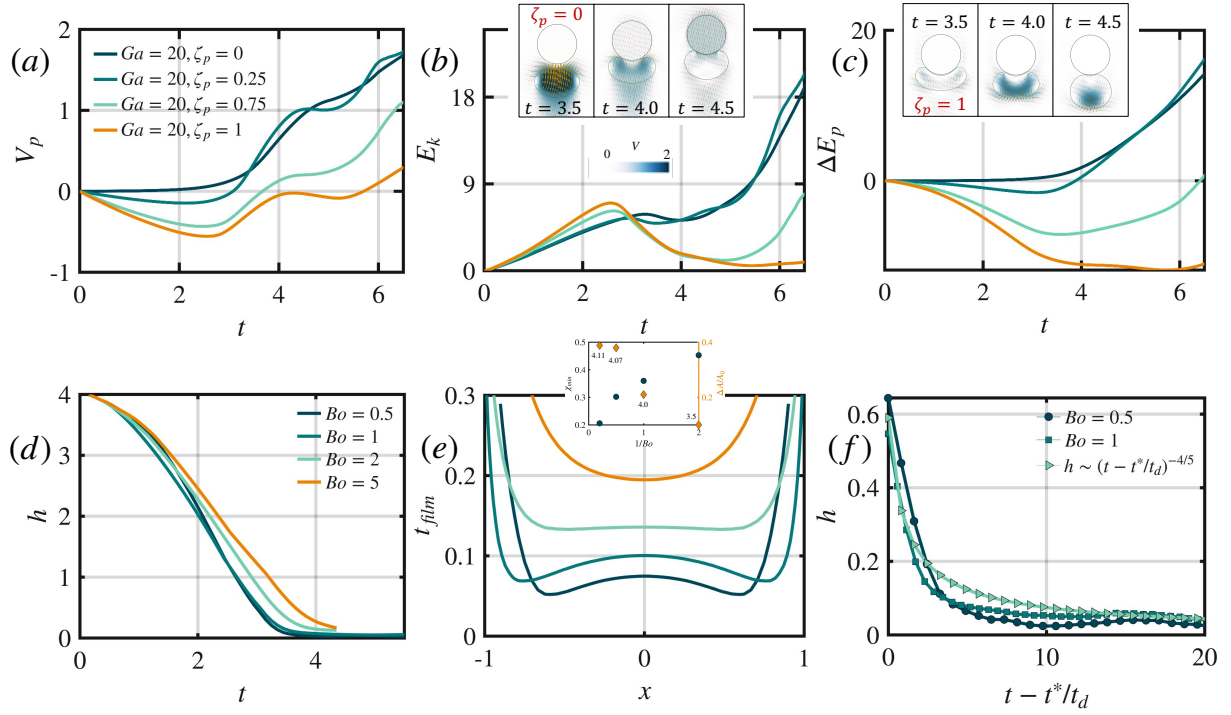


Figure 6.11: In panels (a), (b) and (c), the particle settling velocity, total kinetic energy, and the change in particle potential energy are presented, respectively. These results correspond to when $Ga = 20, Bo = 0.5$ and varying ζ_p . Temporal evolution of the minimum gap thickness $h(t)$ is shown in (d) for $\zeta_p = 1$, $Ga = 20$, and $Bo = [0.5 - 5]$; an enlarged view of the plot in (d) is shown in panel (f), for $Bo = 0.5$ and $Bo = 1$ as at these Bo numbers, the bubble did not rupture. A scaling for the film drainage is provided such that $h \sim ((t - t^*)/t_d)^{-4/5}$. Panel (e) showcases the film thickness profile at $t_{\chi_{min}}$ when varying Bo and maintaining $Ga = 20$ and $\zeta_p = 1$.

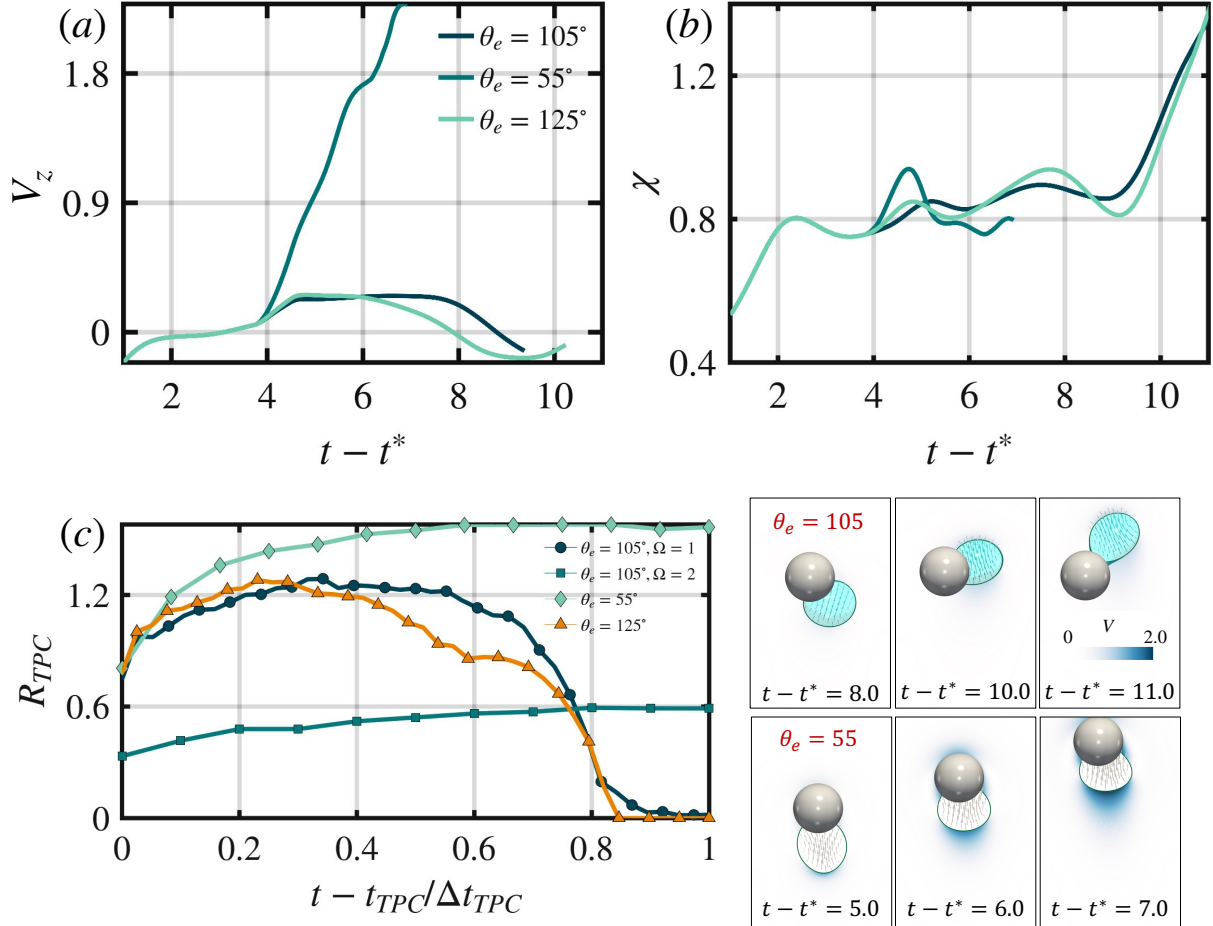


Figure 6.12: This figure showcases the dynamics of the interaction after the formation of the contact line, when $Ga = 10$, $Bo = 0.5$, and $\zeta_p = 1$. In panel (a), the particle's vertical velocity is presented for different particle wettability parameters, which correspond to a base case with $\theta_e = 105^\circ$, and two additional cases with $\theta_e = 55^\circ$, and $\theta_e = 125^\circ$. The figures on the right-hand side correspond to $t - t^*$ from 8 to 11 for the base case and $t - t^*$ from 5 to 7 when $\theta_e = 55^\circ$. Panel (b) showcases the aspect ratio χ for the three different cases. Lastly, panel (c) showcases the temporal evolution of the radius of the contact line R_{TPC} when varying θ_e and Ω . Note that the x -axis is scaled with the contact line time t_{TPC} .

the liquid film thickness profiles in panel (e), and the liquid film ruptures at $t - t^* \approx 2.5$. It can be seen that, unlike the case where $\Omega = 1$, decreasing the particle size leads to the bubble continuing to rise during the film-draining process, which can be seen from the apex position of the bubble in panels (b) and (f) for the two cases. When the film ruptures, the larger bubble continues to push the particle upwards until it reaches the top boundary.

We further consider the effect of increasing Ga and varying ζ_p on the interaction dynamics in Fig. 6.11. Seven different cases are presented, which correspond to $(Bo, Ga, \zeta_p) = (0.5, 20, 1), (1, 20, 1), (2, 20, 1), (5, 20, 1), (0.5, 20, 0), (0.5, 20, 0.25),$ and $(0.5, 20, 0.75)$. In panel (a), the temporal evolution of the particle velocity is presented. Previously, at a Bond number of 0.5, a Galilei number of 10, and a relative particle-to-fluid density contrast of 1, the bubble and the particle remained at relatively the same vertical position throughout the film draining process. This indicates that the bubble and particle experienced minimal vertical displacement relative to each other due to the difference in buoyancy force between the bubble and the particle. When Ga is increased to 20 while maintaining $\zeta_p = 1$, the bubble approaches the particle with a greater velocity compared to when $Ga = 10$. However, the dynamics of the interaction remains consistent with the case when $Ga = 10$, where the magnitude of the velocity of the particle decreases and the particle remains in relatively the same vertical position during film drainage (see panel (c) of Fig. 6.11). In this investigation, we consider the effects of decreasing the relative particle-to-fluid density contrast (ζ_p), which introduces new dynamics into the interaction process. Specifically, a lower ζ_p makes the particle less dense relative to the fluid, increasing its susceptibility to the forces exerted by the bubble. This increased sensitivity results in more pronounced motion reversals and changes in velocity, demonstrating a critical dependence on the density contrast for the overall behavior of the bubble-particle interaction. When ζ_p is decreased, the increased velocity of the bubble causes it to push the particle upwards as the gap distance between them decreases. The extent of flotation of the particle increases as ζ_p decreases. This can be verified by examining panels (a), (b) and (c), which show the particle velocity, the total kinetic energy, and the change in potential energy of the particle, respectively. Specifically, the bubble's kinetic energy becomes significant, imparting momentum to the particle and causing it to reverse its motion. This reversal is similar to the behaviour observed when $\Omega = 2$. As the particle reverses its motion due to the bubble's kinetic energy, the bubble's velocity decreases post-interaction. This deceleration results from the transfer of energy from the bubble to the particle, which leads to a redistribution of momentum. The interaction process for $\zeta_p = [0, 1]$, $Ga = 20$, and $Bo = 0.5$ can be seen in Fig. 6.11.

When considering the temporal evolution of the gap thickness between the bubble and the particle for $Ga = 20$ and $\zeta_p = 1$, a similar general trend is found compared to that shown in Fig. 6.10. Increasing Bo leads to an increase in the surface area between the bubble and the particle, delaying the process of film drainage. However, when comparing Fig. 6.11(d) to Fig. 6.10(a), the bubble ruptured for both $Bo = 2$ and $Bo = 5$ when increasing the impact relative velocity by varying Ga . Panel (e) of Fig. 6.11 shows the film thickness when varying Bo and maintaining $Ga = 20$ and $\zeta_p = 1$ at $t_{\chi_{min}}$. As seen in panel (d) of Fig. 6.6, the film thickness profile indicates an increase in the distance between the bubble and the particle with increasing Bo , and the minimum thickness shifts from the bubble dimple to the centreline. Following a similar scaling method to Fig. 6.10, the minimum film thickness when $Bo = 0.5$ and $Bo = 1$ scales as $h \sim (t - t^*/t_d)^{-4/5}$.

For head-on collisions with relatively small Bo numbers, a contact line forms between the bubble and the particle after liquid film drainage. In Fig. 6.12, the evolution of the contact line dynamics and the effect of particle wettability on the overall dynamics is studied. Three different equilibrium contact angles are considered, and they are $\theta_e = (55, 105, 125)$ for $\Omega = \zeta_p = 1, Ga = 10$, and $Bo = 0.5$. First, panel (a) showcases the particle vertical velocity for the three cases. When $\theta_e = 55$, the particle velocity is seen to increase significantly post contact line formation, which indicates that the bubble has attached to the particle and is pushing it upwards. When increasing θ_e to 105° or 125° , the particle velocity is not as significantly affected, indicating the bubble is attempting to minimise its contact area with the particle. In panel (c), the radius of the contact line R_{TPC} is shown when varying θ_e and Ω . When $\theta_e = 55^\circ$, the contact line initially expands, and during the expansion, the bubble vertically deforms which leads to a peak in the aspect ratio χ at $t - t^* \approx 4.8$ (panel (b)). The contact line radius then maintains the same size as it floats with the particle until reaching the top boundary. When increasing θ_e , the contact line radius initially expands, however, the bubble ‘slides’ across the particle and attempts to minimise the contact area. This leads to a decrease in the contact line radius as the bubble moves to the particle’s apex, and the bubble then detaches due to buoyancy and continues to rise. The bubble detaches at $t - t^* \approx 9$ when $\theta_e = 105^\circ$ and $\theta_e = 125^\circ$, with a small part of the bubble still attached to the particle surface. When decreasing the particle size ($\Omega = 2$) and maintaining $\theta_e = 105^\circ$, the radius of the contact line expands during contact. However, due to the particle’s upward velocity induced by the bubble during the initial interaction, the bubble and the particle continue to rise and the contact line remains relatively the same size. It is crucial to note that the initial radius of the contact line indicates the position at which the contact line forms, such that the dimple radius has a direct influence on the dynamics of the contact line.

6.3.2 Off-centre bubble-particle interactions

Here we consider bubble-particle interactions that do not correspond to head-on collisions. These are initiated by introducing a horizontal deviation δ in the initial bubble position. In this section, we study the dynamics associated with $\delta = [0.25, 0.5, 1]$ and keep $(Ga = 10, \zeta_p = 1)$ fixed. In Fig. 6.13, the spatio-temporal evolutions of the interaction between the bubble and the particle are presented for $Bo = 0.5$ (top two rows) and $Bo = 5$ (bottom two rows), and $\delta = 1$. The background field shows the logarithm of the viscous dissipation function ξ in the fluid. When initiating an offset between the bubble and the particle, it can be seen in Fig. 6.13 that for $Bo = 0.5$, the bubble initially rises in a similar fashion as observed with the in-line collisions, but the dimple at the apex of the bubble forms on the side of the bubble rather than at the centreline. This causes the bubble to shift its velocity towards the other side (as seen in the glyphs) as it deforms during the interaction process. A liquid film forms between the bubble and the particle at the side of the bubble, at which point we have the largest dissipation of energy. The bubble tends to exhibit a ‘sliding’ motion, which is similar to the drafting-kissing-tumbling (DKT) regime found by Zhang et al. [63] between two bubbles rising in line. The bubble is then seen to continue its rise as it recovers its original spherical shape, which can be seen at $t = 5.5$ and $t = 6$. This can also be observed by the change in the surface area plot in Fig. 6.14(b), where the change in surface area decreases after the interaction with the particle.

Upon further increasing Bo to $Bo = 5$, a similar initial interaction process is observed such that the bubble rises with an ellipsoidal shape and a dimple forms on the side of the bubble rather than at the centreline. However, due to the large deformations associated with this Bo value, it can be seen that although a DKT scenario is found, the side of the bubble associated with the impact forms a ‘tail’ ($t = 4.5$ – 5.5). As the tail forms, we have a sharp increase in the bubble interfacial area and energy dissipation, while the centre of mass of the bubble continues to rise as the total kinetic energy increases (see Fig. 6.14(a)). The tail of the bubble then retracts to its centre of mass ($t = 6$ in Fig. 6.13) and continues to rise, and the particle continues to settle.

From Fig. 6.14(d) it can be seen that upon increasing Bo , the deviation in the particle settling trajectory is not as affected as for low Bo . This is associated with the significant deformation of the bubble, which tends not to affect the x -component of the particle velocity as much as the sliding motion of the bubble observed for $Bo = 0.5$. Furthermore, when fixing $Bo = 0.5$ and varying δ between 0.25–0.5, Fig. 6.14(e–f) shows that the particle trajectory is affected more by decreasing the value of δ . For $\delta = 0.25$ and $\delta = 0.5$, the particle’s settling velocity (see Fig. 6.14(c)) decreases during the initial interaction

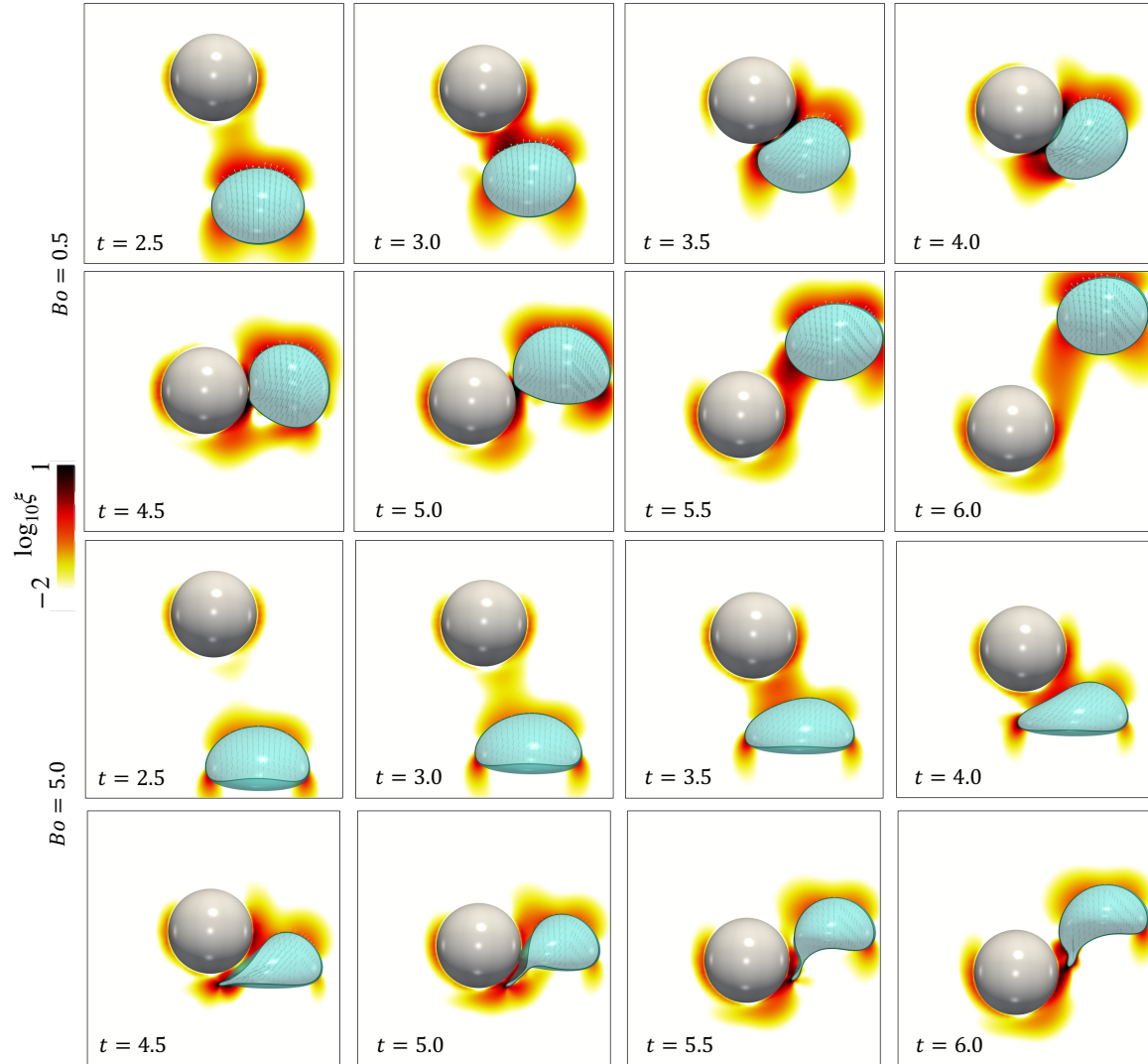


Figure 6.13: Spatio-temporal evolution of off-centre bubble-particle interaction dynamics with $Ar = 10$, $Ga = 10$, and an initial bubble location offset of $\delta = 1$. The results shown in the top and bottom two rows were generated with $Bo = 0.5$ and $Bo = 5$, respectively. The contours are of the logarithm of the viscous dissipation function $\log_{10} \xi$ in the fluid. The bubble is shown with glyphs of the velocity to illustrate the relative motion of the bubble at different time-steps. The snapshots are shown between $t = 2.5$ and $t = 6$ in time-increments of $\Delta t = 0.5$.

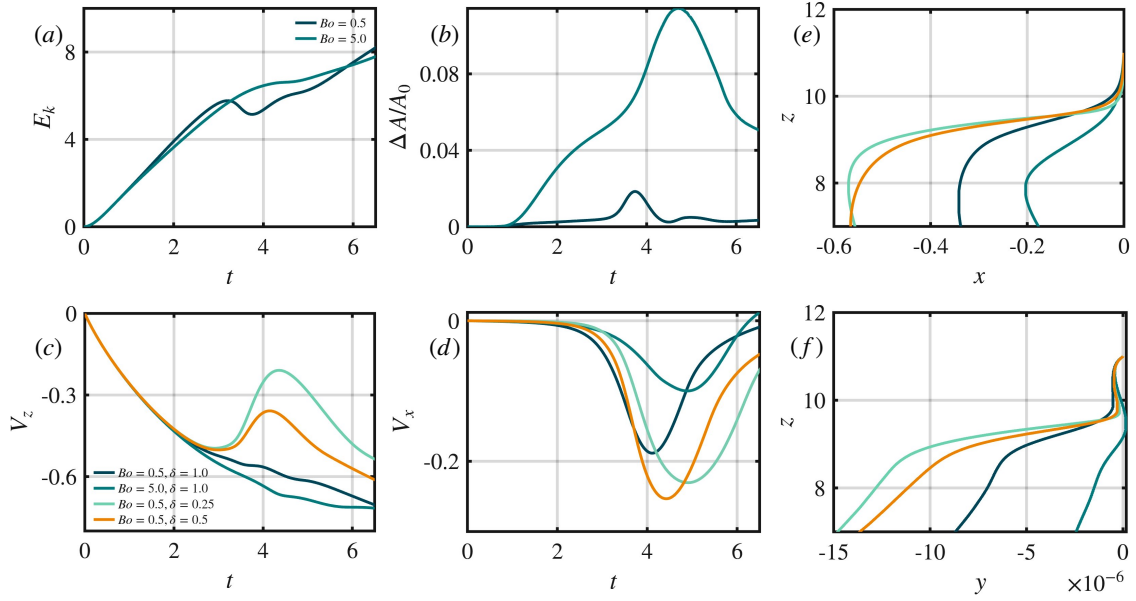


Figure 6.14: Temporal evolution of the total kinetic energy, and the change in bubble surface area are shown in (a)-(b), respectively, for off-centre bubble-particle interactions with $(Bo, Ga, Ar, \delta) = (0.5, 10, 10, 1)$ and $(5, 10, 10, 1)$. Panels (c) and (d) show the temporal evolution of the settling velocity, and the x -component of the particle velocity, respectively. In panels (e) and (f), the side view of the particle trajectory with respect to the x -axis and the y -axis are presented, respectively.

process. Although the decrease in settling velocity is more pronounced as δ decreases, i.e., approaching the case of in-line bubble-particle interactions, the variation in the x -component of the velocity is more pronounced when $\delta = 0.5$ compared to $\delta = 0.25$ (see Fig. 6.14(f)). This leads to the particle trajectory being rather similar when $\delta = 0.25$ and 0.5 (see Fig. 6.14(e)).

6.4 Concluding remarks

This chapter considered the interaction between a freely-rising deformable bubble and a freely-settling particle in a quiescent, Newtonian background fluid. The considered non-dimensional parameters were the bubble Bond and Galilei numbers, the particle Archimedes number, governed by the solid-fluid density contrast, and the size ratio between the bubble and the particle. The results highlighted the spatio-temporal evolution of the bubble shape during the interaction process, the bubble aspect ratio as a measure of its deformation, the liquid film thickness, and an energy analysis of the system. When considering the bubble shape, it was found that increasing the Bond number led to more severe bubble deformations, leading to bubble rupture and its penetration by the parti-

cle. This is caused by the north and south poles of the bubble coalescing as a result of the intensity of the deformation. When the Bo number is relatively low, the interaction includes the formation of a liquid film between the bubble and the particle, which is associated with the dissipation of kinetic energy. When decreasing ζ_p , the buoyancy force of the bubble exceeds that of the particle, and the bubble can lift the particle upwards if the approach velocity of the bubble is considerably larger than that of the particle. However, if the particle and the bubble approach velocities are similar in magnitude, the initial interaction process is associated with the dissipation of kinetic energy which causes the bubble and the particle to remain at their interaction position as the liquid film drains. The study also considered the temporal evolution of the minimum gap thickness ($h(t)$) between the bubble and the particle and found that increasing Bo led to an increase in surface area in the gap region, further delaying the film-draining process. The effect of particle wettability on the contact line dynamics was also considered, such that the bubble remains attached to the particle surface at lower θ_e and slides away at larger θ_e .

Outokesh et al. [191] recently investigated experimentally a setup that is closely related to the numerical configuration considered here. Their results highlighted the emergence of four distinct regimes, namely: (i) the shuttling regime, where the bubble acts as a carrier for the particle by effectively reducing its inertia; (ii) the bouncing regime, where the particle rebounds from the interface, consistent with the behaviour observed here at $Bo = 2$; (iii) the penetration regime at high Bo , in agreement with the findings reported here at $Bo = 5$; and (iv) the flotation regime, which is commonly reported in industrial settings involving small hydrophobic particles. Overall, these recent experimental observations are in close alignment with the numerical results presented here and further support the findings in this chapter. From a numerical standpoint, fully three-dimensional simulations of this process are computationally expensive, and a systematic mapping of all regimes across parameter space is therefore beyond the scope of the present work. Instead, the results reported here are intended as a stepping stone for future studies of bubble-particle interactions, providing a baseline set of validated observations and modelling choices that can be extended to broader conditions. This direction has also gained traction in the literature since the related manuscript for this chapter was published, further motivating continued investigation. In this context, the present high-fidelity simulations may also provide useful validation data for reduced-order models (ROMs), which could incorporate bubble-particle interaction effects into larger scale descriptions of multiphase flows without resolving the full interfacial dynamics in every interaction event.

A complex situation arises when introducing an offset between the bubble and the particle initial positions. In this study, an offset is only considered for the bubble initial

position in the horizontal direction at constant Archimedes and Galilei numbers. For low Bond numbers, a sliding motion of the bubble was observed as it approached the particle, causing the bubble to push the particle away from its original settling trajectory. However, with increasing Bond number, the bubble deformation is seen to be much more severe such that the bubble centre of mass continues to rise with the formation of a tail in the particle's proximity. The tail then retracts, the bubble continues to rise, and the trajectory of the particles is not affected as significantly.

This work has considered one viscosity and density ratio between the bubble and the background fluid $\lambda = \mu_l/\mu_b = 100$ and $\beta = \rho_l/\rho_b = 1000$. Possible avenues for future work may include the effects of varying the viscosity and density ratios, considering a larger difference between the particle and bubble sizes, introducing asymmetric particle shapes, and the effect of density stratification in the background fluid. Furthermore, the effects of surface mobility of the bubble on the interaction process, introducing surfactants into the system, for example, presents an interesting avenue of future work due to its relevance for industrial processes. All of these configurations may lead to different interaction dynamics between the bubble and the particle. Lastly, this work has considered the interaction between a single rising bubble and a single settling particle; however, the collective effect of the interaction between a rising bubble, or a group of bubbles, in the presence of a particle suspension remains an area for further exploration. Recently, Zeng et al. [120] have tackled the problem of rising bubbles capturing hydrophobic particles in a Newtonian fluid using a front-tracking framework. This is of interest because the problem is receiving increasing attention in the literature due to its many applications, yet it remains comparatively underexplored relative to more canonical cases. Their numerical framework also employed a GNBC model to model the moving contact line, in a manner similar to the approach adopted in the present work. Additional works are recommended to investigate this broad topic, for example, by exploring the role of surfactants and coalescence as the bubble volume fraction increases.

6.5 Resolution tests

In this section, a resolution test is presented for the case when $(Bo, Ga, Ar) = (0.5, 10, 10)$ in Fig. 6.15. Two different mesh resolutions are considered, and they correspond to $\Delta x/R = 1/24$ and $\Delta x/R = 1/32$. Furthermore, three different mesh resolutions are considered in panel (d) for the case of $Bo = 5.0$ and $Ga = 10$, where a resolution of up to $\Delta x/R = 1/64$ is presented (doubling the resolution). When considering the distance

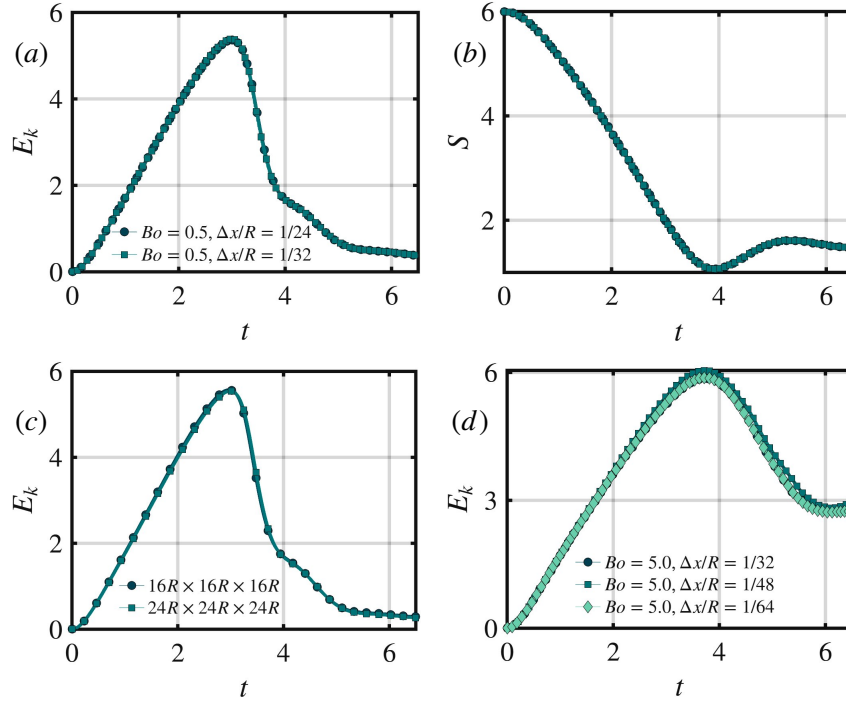


Figure 6.15: The top two panels (a) and (b) show the total kinetic energy of the system and the distance between the particle south pole and the bubble south pole (S), at two different resolutions for $Ga = 10$, $Bo = 0.5$, and $\zeta_p = 1$, respectively. Panel (c) shows the temporal evolution of the total kinetic energy when increasing the domain size for the same case. It can be seen that increasing the domain size leads to no difference in the results. Panel (d) shows the total kinetic energy for different mesh sizes for $Ga = 10$, $Bo = 5.0$, and $\zeta_p = 1$, up to a resolution of $\Delta x/R = 1/64$. The results show that the domain size and mesh resolution utilised in this work is sufficient to capture the dynamics of the interaction between the bubble and the particle.

between the particle south pole and the bubble south pole, and the total kinetic energy of the system, an excellent agreement is found between the two mesh resolutions. The most difficult part to resolve is the film thickness. The lower resolution RMSE compared to the higher resolution is approximately 0.5%, which is acceptable considering the higher resolution is the coarsest mesh utilised in this study. In panel (c), a domain size independence test is performed when $Bo = 0.5$ and $Ga = 10$, by increasing the domain size to $24R \times 24R \times 24R$. The results show that when increasing the domain size, there is no difference in the attained result, further increasing our confidence in the numerical setup.

Chapter 7

Conclusions and future outlooks

This thesis has aimed to advance the fundamental understanding of particle dynamics in conditions representative of those experienced by microplastics, with a focus on density-stratification, particle geometry, particle–particle interactions, and multiphase effects such as bubble–particle interactions. To do this, the work relied on particle-scale direct numerical simulations (DNS) that resolve the flow around individual particles. The problems studied build on single-body dynamics in homogeneous fluids, where many mechanisms are now well established, and extend towards more complex settings where stratification, particle proximity effects, and interfaces introduce additional physical pathways that remain less well characterised.

The literature reviewed in Chapter 2 of this thesis shows that in homogeneous fluids, particle dynamics are now reasonably well understood across a wide range of Reynolds numbers, with established links between wake structure, path stability, and the resulting hydrodynamic forces. Bubble motion in homogeneous Newtonian fluids is similarly governed by competing effects of buoyancy, viscous resistance, inertia, and surface tension, which together determine rise speed, deformation, and wake development. Depending on the controlling dimensionless groups, bubbles can remain nearly spherical or transition through a range of deformed shapes, with wake-driven path instabilities emerging in many regimes. In stratified fluids, new behaviour arises through coupling between buoyancy and diffusion. These couplings can alter trajectories and residence times and can promote unsteady motion, including oscillatory dynamics reported in the literature. A related class of problems concerns translating bodies interacting with horizontal immiscible interfaces, where quasi-static behaviour can often be understood through force balances, while increasing inertia leads to pinch-off, entrainment, and more complex, sometimes fully three-dimensional, outcomes. Taken together, this background highlights that while

the broader literature on particle and bubble dynamics is extensive, configurations that combine particle geometry and particle–particle interactions in density-stratified fluids, as well as bubble–particle interactions, remain comparatively underexplored. These gaps motivated the problems addressed in this thesis.

A consistent numerical framework presented in Chapter 3 was applied across the thesis. For the multiphase flow simulations involving deformable interfaces, a Lagrangian–Eulerian formulation based on the Level Contour Reconstruction Method (LCRM) was employed. The multiphase methodology was described alongside the assumptions and implementation choices adopted in the present work and positioned with respect to alternative approaches used elsewhere in the literature. Rigid particles were handled using a fictitious domain method, and benchmark tests were presented within each chapter in regimes appropriate to the specific problems studied.

In Chapter 4, the first set of results focused on isolated bodies in homogeneous and density-stratified fluids, with particular attention to how geometry affects wake dynamics and stability. Benchmark tests for settling isolated spheres in both homogeneous and stratified fluids showed excellent agreement with established results in the literature, providing confidence in the solver and its coupling to stratification. The chapter then examined the rise dynamics of solid and annular discs in homogeneous and linearly stratified fluids at moderate Reynolds numbers. For impervious discs in homogeneous fluid, the numerical results matched well with available experimental measurements of the homogeneous drag coefficient, C_D^H . Introducing a central perforation produced a clear stabilising effect for the conditions considered, yielding a transition from fluttering motion to rectilinear rise at moderate Archimedes numbers, consistent with prior experimental observations that holes can suppress path instabilities. This stabilisation was quantified using the circulation by separating the contributions from the primary and secondary counter-rotating vortex rings in the wake, which clarified how perforation alters the wake structures that drive lateral motion. In linearly stratified cases, the analysis showed that wake structure is modified in a way consistent with earlier studies of bodies moving through stratified ambients. In particular, the rise of discs generated an additional detached toroidal vortex in the wake, attributable to baroclinic vorticity production. Under sufficiently strong stratification, the bodies underwent an orientational instability, transitioning from a broadside-on configuration to an edgewise orientation, which is a known behaviour for discs and spheroids in stratified fluids. A key finding of this chapter is that the size of the perforation modifies the onset and development of this instability. Increasing the perforation ratio d/D_D delayed the onset of reorientation and reduced the threshold velocity at which reorientation begins. The growth rate of the instability

decreased with increasing d/D_D , and the results support an interpretation in which perforation changes the alignment and coupling between the disc and the stratification-induced vortex plume, thereby weakening the torque that drives the instability. These results are relevant to oceanic settings where stratification modifies both wake dynamics and body orientation, and they suggest that permeability, used here as a proxy for weathered fragments, can change wake strength and delay reorientation near pycnoclines. This implies potential changes in residence time and lateral dispersion for particles moving through stratified layers, which matters for interpreting transport pathways of microplastics and related particulate material.

The thesis then examined particle–particle interactions in stratified fluids in Chapter 5, first through the dynamics of an in-line particle pair and then through sparse clusters. For a spheroidal pair settling in-line in a linearly stratified fluid at $Ar = 4.65$, the results revealed a characteristic sequence: an initial drafting phase where the trailing particle is drawn into the wake of the leading particle, followed by a separation phase driven by stratification effects. During drafting, a reverse jet formed behind the trailing particle as the pycnoclines were restored towards their neutrally buoyant configuration, and this transient jet altered the near-wake flow. As separation began, a secondary jet developed in the gap between the leading and trailing particles, and this feature played a central role in reorienting the trailing particle. Reorientation was more pronounced for oblate spheroids than for prolate spheroids. In the oblate cases, the secondary jet caused the trailing particle to tilt and escape the leading particle’s wake, producing an asymmetric side-escape regime. Increasing the initial separation distance led to an earlier onset of the secondary jet in the gap region. Additional oblate aspect ratios at large Sc showed that side escape persists but with reduced lateral drift as the aspect ratio increases, indicating a clear shape dependence in how stratification-driven effects translate into reorientation and lateral motion. Further simulations at smaller Sc showed that the transient jet strength decreases as diffusion increases, and in the present parameter range this can suppress reorientation altogether. Finally, varying the Archimedes number at moderate Fr and Sc indicated that several regimes resemble those reported for homogeneous fluids, which helps separate stratification-driven behaviour from wake-mediated interaction mechanisms that persist across both settings.

For particle clusters, the simulations showed that stable density-stratification can fundamentally alter both the effective particle–particle interactions and the resulting cloud evolution. For clusters initialised with small separations, stratification promoted an effective lateral attraction that suppressed transverse spreading compared with homogeneous cases, leading to more laterally aligned configurations as particles settled. This appeared

as a clear reduction in the growth of transverse variance at late times as Fr decreases. In configurations with a sharp density transition, the crossing of the transition layer was characterised by a strong reduction in the vertical speed $|V_z|$, and the transverse variance decreases during the crossing, indicating a transient contraction, before increasing again once entrained light fluid returned towards its equilibrium level beneath the transition. Parameter variations showed that stronger stratification (larger Γ) and weaker scalar diffusion (larger Sc) intensify the slowdown by increasing the effective local stratification experienced by the cluster, while a thicker transition layer (larger H) smooths the response. Although stratification tended to preserve lateral coherence, increasing N_p could still favour vertical reorganisation through wake-mediated interactions, producing leading and trailing subgroups, and this tendency is expected to be stronger in polydisperse suspensions. Preliminary cases also suggested the possibility of lateral drift of the cluster centre of mass at sufficiently small Fr , consistent with reports of horizontal migration of non-spherical bodies in linearly stratified fluids. These findings indicate that stratification can suppress lateral dispersion while opening new pathways for vertical structuring and, in some cases, lateral drift, which is important for interpreting transport and mixing associated with particle-laden flows in stratified environments.

The final part of the thesis studied bubble–particle interactions in Chapter 6, focusing on a freely rising deformable bubble interacting with a freely settling particle in a quiescent Newtonian liquid. The governing parameters included the bubble Bond and Galilei numbers, the particle Archimedes number set by the density contrast, and the bubble-to-particle size ratio. The simulations resolved the evolution of bubble shape, quantified deformation through the bubble aspect ratio, tracked the development and evolution of the liquid film between the bubble and the particle, and used an energy-based analysis to interpret the interaction outcomes. A central result is that increasing Bo leads to more severe bubble deformation, and sufficiently strong deformation can cause bubble rupture and penetration by the particle, associated with the approach and coalescence of the bubble poles. At lower Bo , the interaction is characterised by the formation of a liquid film that dissipates kinetic energy and introduces a drainage controlled time scale that can dominate the dynamics. The balance between bubble and particle buoyancy, together with the relative approach speeds, further determined whether the bubble could lift the particle upward or whether the interaction could become arrested while the film drains. The simulations also showed that increasing Bo can increase the surface area in the gap region and delay the film-draining process. Particle wettability introduced an additional control through contact line dynamics, with lower equilibrium contact angles θ_e favouring attachment of the bubble to the particle and higher angles promoting sliding away.

These results connect well with recent experimental work on closely related configurations, which has identified distinct regimes including shuttling, bouncing, penetration, and flotation. The present simulations reproduced key features consistent with those regimes, including bouncing at $Bo = 2$ and penetration at $Bo = 5$, and they provide complementary information on the resolved flow field, film evolution, and energy pathways that are difficult to measure directly. The thesis also explored the effect of an initial horizontal offset of the bubble relative to the particle. The bubble exhibited a sliding motion during approach and could push the particle away from its original settling trajectory. While a complete regime map would require extensive three-dimensional parameter sweeps that are computationally prohibitive, the results in this thesis provide a validated baseline and a set of mechanisms that can guide future investigations.

Across the thesis, a consistent picture emerges: stratification and deformable interfaces can substantially alter particle motion by changing the local force balance, wake structure, and interaction dynamics. For isolated bodies, stratification generated baroclinic wake structures that could drive orientational instabilities, while perforation modified the coupling between the body and its wake. For interacting particles, stratification produced return flows that influenced separation, reorientation, clustering, and lateral dispersion. In bubble–particle systems, the deformable interface introduced additional mechanisms, including film drainage and contact line motion, that influenced the interaction outcome.

The environmental picture motivating these results is that microplastics are not confined to the sea surface. Although many fresh plastic fragments are positively buoyant, their apparent density and surface properties evolve through weathering, aggregation with organic matter, and biofouling, altering their effective density and therefore their tendency to rise, settle, or remain suspended near density interfaces. Vertical transport can therefore carry particles away from the surface and into stratified regions of the water column, where sharp density gradients such as seasonal thermoclines, coastal pycnoclines, estuarine haloclines, and density transitions below the surface mixed layer can influence their residence time and dispersion. These interfaces commonly occur over depths ranging from a few metres in coastal and estuarine environments to tens or hundreds of metres in the open ocean, while the gradients themselves may be much thinner than the surrounding water column.

The parameter ranges considered in Chapters 4 and 5 can be related to field and laboratory conditions through the Froude number. As discussed by Zhang et al. [14], whether a buoyancy-driven body reaches $Fr = O(1)$ depends on the combined effects of stratification strength, body size, vertical velocity, and excess density, rather than

on the buoyancy frequency N alone. For a high-Reynolds-number Argo-float example, they considered a background stratification with $N \simeq 0.015 \text{ s}^{-1}$ and estimated that the Froude number changes from $Fr \simeq 12$ at a vertical speed of approximately 9.1 cm s^{-1} to $Fr \simeq 1.32$ at approximately 1 cm s^{-1} , with the latter case corresponding to a much larger stratification-induced drag enhancement. In laboratory studies of small low-Reynolds-number particles, comparable $Fr = O(1)$ conditions are reached using much stronger stratification, with N typically in the range $1.5\text{--}3 \text{ s}^{-1}$ and in some cases up to 7.2 s^{-1} , because the particles must experience strong density gradients over the limited height of laboratory tanks.

More directly relevant to natural particulate transport, Zhang et al. [14] identified marine-snow aggregates in upper-ocean and estuarine haloclines as low-Reynolds-number particles for which $Fr = O(1)$ can occur because the excess density is very small while the local stratification is strong. They noted that while a representative open-ocean value is $N \simeq 0.01 \text{ s}^{-1}$, strong haloclines can reach $N \simeq 0.04\text{--}0.07 \text{ s}^{-1}$, with values up to approximately 0.2 s^{-1} reported in estuaries and fjords. For porous marine-snow aggregates with $\Delta\rho/\rho_0 \simeq 1.9 \times 10^{-4}$, they estimated $Fr \simeq 1.25$, providing a concrete environmental example in which stratification can substantially modify settling, residence time, and accumulation. This interpretation is consistent with the field observations of MacIntyre et al. [15], who reported enhanced marine-snow concentrations at density discontinuities in the water column, and it provides a mechanistic context for how marine snow, planktonic aggregates, and microplastic-organic aggregates may be retained or concentrated near pycnoclines and haloclines.

Zhang et al. [14] also noted that $Fr = O(1)$ behaviour can arise when particles or drops cross sharp immiscible interfaces between fluids of similar viscosities, as studied by Pierson and Magnaudet [102] and Pierson and Magnaudet [103]. In such cases, the relevant restoring effect is associated with the interfacial density jump, and the particle motion can be strongly altered by interface deformation, capillary effects, and the entrainment of a long fluid tail. Their example of a sphere crossing an oil/water–glycerine interface showed a pronounced reduction in settling speed as the interface was deformed and stretched, illustrating that sharp material interfaces can influence particle transport in a manner analogous to strong stratified layers.

The simulations in this thesis isolate the particle-scale mechanisms that can operate when such particles encounter these layers: Chapter 4 shows how fragment geometry and porosity-like features alter wake strength and reorientation near stratification; Chapter 5 shows how stratification changes particle–particle interactions, clustering, and dispersion

as particles settle through or near density gradients; and Chapter 6 shows how rising bubbles can lift, deflect, or fail to capture particles depending on deformability, inertia, and wettability. In this sense, the thesis does not attempt to reproduce a complete oceanic flow, but identifies mechanisms that can influence residence time, accumulation, vertical redistribution, and lateral spreading of microplastics within and around stratified layers.

Several physical effects that are important in practical settings were not included in the present scope, including surfactants and variable surface mobility for bubbles, more complex background flows such as turbulence and shear, more diverse particle shapes, and, in the bubble–particle chapter, the additional coupling that would arise if the ambient were density-stratified. Some future directions follow naturally from this work. For bubble–particle interactions, it would be valuable to vary the viscosity and density ratios, explore a wider range of bubble–particle size ratios, and examine asymmetric and more realistic particle shapes. Including surfactants and surface mobility would allow direct study of how film drainage, contact line motion, and regime changes under conditions relevant to industrial and environmental applications. Extending from single interactions to collective behaviour, studies of bubbles interacting with particle suspensions, and multiple-bubble systems, would help bridge towards realistic multiphase particulate flows. For stratified particulate transport, scaling up to larger numbers of non-spherical particles, including polydispersity and porosity proxies, would clarify how the mechanisms identified for pairs and sparse clusters translate to more complex suspensions.

In conclusion, this thesis has shown that density stratification, particle geometry, particle–particle interactions, and deformable interfaces can produce particle dynamics that differ qualitatively from those observed in homogeneous fluids. By resolving these complexities at the particle scale and linking them to identifiable mechanisms, the thesis provides a basis for improved interpretation and modelling of particulate transport in stratified and multiphase environments, with direct relevance to microplastics and related geophysical flows.

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