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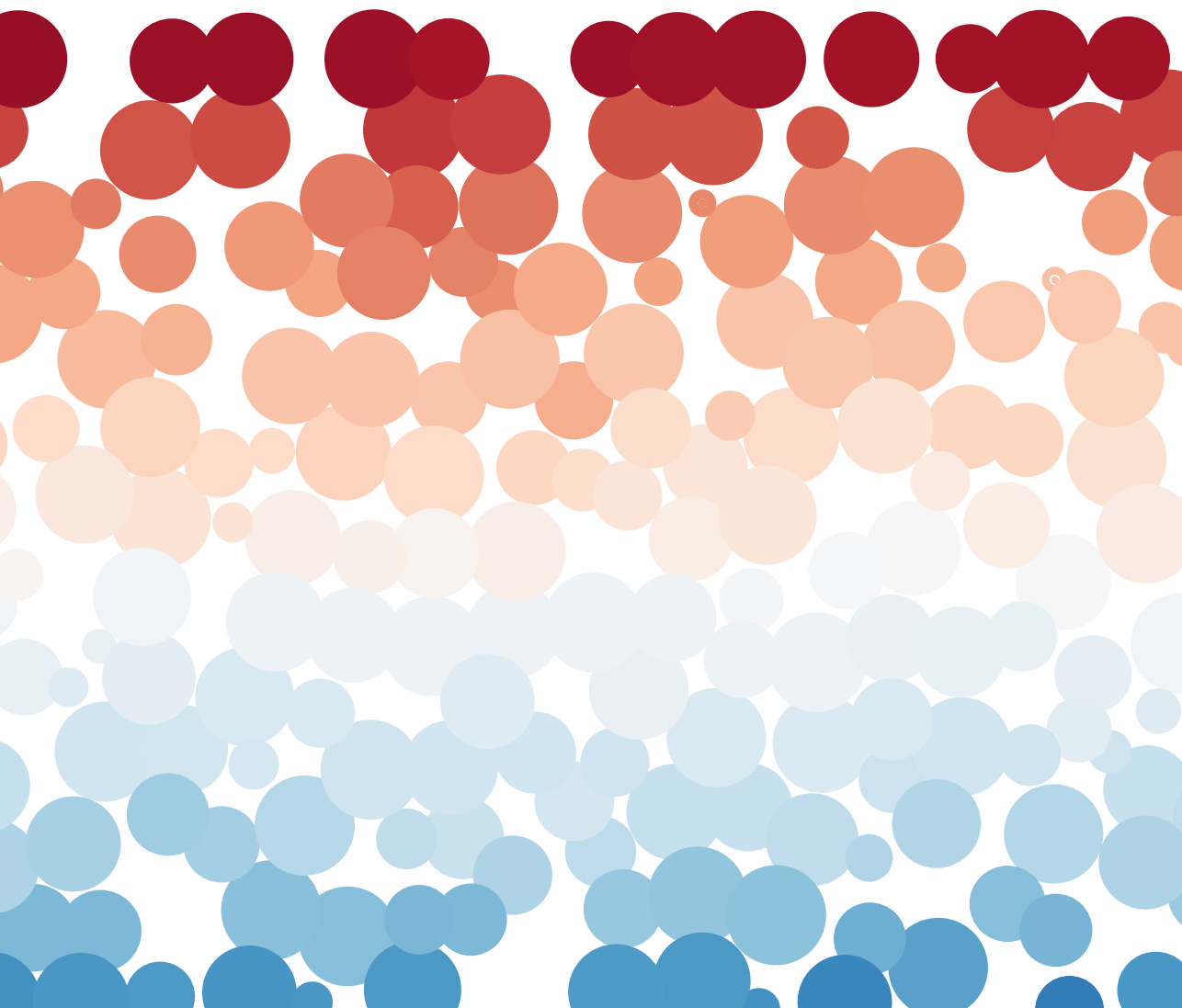
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Rheology and sedimentation of dense suspensions in confined geometries

Insights from particle-resolved direct
numerical simulations

Wouter Peerbooms



Rheology and sedimentation of dense suspensions in confined geometries

Insights from particle-resolved direct numerical simulations

Dissertation

for the purpose of obtaining the degree of doctor
at Delft University of Technology
by the authority of the Rector Magnificus,
Prof. dr. ir. H. Bijl,
chair of the Board for Doctorates
to be defended publicly on
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by

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Keywords: rheology, dense suspensions, sedimentation, shear flow, pressure-driven flow, 3D printing, liquid deposition modeling, direct numerical simulations

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Contents

Summary	v
Samenvatting	ix
1 Introduction	1
2 Viscous sedimentation of dense suspensions in narrow vertical tubes	17
2.1 Introduction	18
2.2 Governing equations and contact model	24
2.3 Numerical method and computational setup	25
2.4 Results and discussion	28
2.4.1 Settling of a single sphere	28
2.4.2 Sedimenting suspensions.	29
2.5 Conclusions	45
3 Interparticle friction in sheared dense suspensions: Comparison of the viscous and frictional rheology descriptions	55
3.1 Introduction	56
3.2 Methods	60
3.2.1 Governing equations and contact model	60
3.2.2 Numerical method and computational setup	62
3.2.3 Statistical averaging	63
3.3 Results	65
3.4 Conclusions	83
3.A On the normalization with the normal stress in the frictional rheology framework.	85
4 Transient behavior and steady-state rheology of dense frictional suspensions in pressure-driven channel flow	93
4.1 Introduction	94
4.2 Methods	100
4.2.1 Governing equations and contact model	100
4.2.2 Numerical method and computational setup	101
4.2.3 Statistical averaging	103
4.3 Results and discussion	105
4.3.1 Particle migration	105
4.3.2 Steady-state rheology	113
4.4 Conclusions	132
4.A Example of determination of different flow regions for calculation of the PPDFs	135
4.B Example of local relative viscosity calculation	135

5	Printability of dense suspensions in Liquid Deposition Modelling	141
5.1	Yield stress	143
5.2	Regime maps	146
5.3	Pressure drop	147
5.4	Suspension stability	150
5.5	Application to UV-LDM	151
5.6	Concluding remarks	152
6	Conclusions and Recommendations	155
6.1	Conclusions	156
6.2	Recommendations	158
	Acknowledgments	163
	Curriculum Vitæ	165
	Scientific Contributions	167

Summary

Solid-liquid suspensions are abundant in our daily lives, in nature, and in industry. The industrial application that we focus on in this work is extrusion-based 3D printing, where suspensions can be used to print for instance: food, metal, or energetic materials. When printing energetic materials, performance requirements dictate that the solid content should be as high as possible. This high solid load creates a challenge to maintain flowable conditions. Additionally, this high volume fraction can create problems with blocking of the nozzle if a contraction is used at the end. Next to the flowability, the homogeneity of the suspension plays an important role, where shear stresses and gravity tend to cause an inhomogeneous microstructure. These aspects relate to the suspension rheology, i.e., the response of the suspension to imposed stress or strain. A good understanding of the rheology is critical to be able to design, optimize, and use printing systems and compositions for energetic materials. The goal of this research is to gain more insight into and to improve modeling of the rheology of dense suspensions for the application in UV-assisted Liquid Deposition Modeling.

In the printing process, 4 different stages can be distinguished: (1) stationary suspension in the reservoir and tubes of the printer when idle, (2) suspension flowing through the supply tube of the printer when active, (3) suspension flowing through the nozzle contraction, and (4) suspension deposited on the printing platform. We employed particle-resolved Direct Numerical Simulations (PR-DNS) to study the suspension rheology under conditions that mimic stages (1) and (2) of the printing process. In the PR-DNS, the full Navier-Stokes equations are solved for the fluid phase, combined with the Newton-Euler equations for the motion of the particles, including a frictional soft-sphere collision model for particle collisions and prolonged contacts. A computationally efficient Immersed Boundary Method is employed for the fluid-solid coupling.

We started our study by simulating dense suspensions sedimenting in narrow tubes in the viscous regime. This flow condition mimics stage (1) of the printing process. We studied both the settling of a single particle and the sedimentation of dense particle suspensions in the volumetric concentration range of $0.05 \leq \phi_b \leq 0.3$. The influence of confinement was investigated for the range of $D/d = 2 - 11$, where D and d are the tube and particle diameter, respectively. By analysing the sedimentation dynamics in terms of, among others, the mean and root-mean-square (rms) particle velocities, the radial particle distribution, particle dispersion characteristics and particle clustering in the vertical direction, we obtained both a clear picture of the macroscopic suspension behavior as well as insight in the underlying suspension microstructure. We found that the mean sedimentation velocity in narrow tubes can be accurately described by a modified Richardson-Zaki correlation for hindered settling in which the terminal velocity for a single particle settling in free space is replaced by the Francis correlation for settling in a narrow tube. For the ratio of the particle rms to the mean sedimentation velocity, we found a clear scaling with $\phi_b^{1/3} (D/d)^{2/3}$, with a deviation from this scaling for $D/(d\phi_b^{-1/3}) \lesssim 2.5$. Furthermore,

for $D/d \geq 6$ and $\phi_b = 0.2$, we observed a peak in the radial velocity distribution at a distance of $\approx 1.4d$ from the tube wall, that resembles a streaming-like behavior with elongated dense particle clusters sedimenting faster than the surrounding more dilute regions. For the studied particle concentration and tube-to-particle diameter ratios, we concluded that confinement has a strong influence on the sedimentation behavior, with a change in the scaling behavior observed for $D/(d\phi_b^{-1/3}) \lesssim 2.5$ and $D/d \lesssim 4$.

Second, we studied the rheology of dense suspensions in simple shear flow to get a better insight into the modeling of suspension rheology for stage (2) of the printing process. We compared two different frameworks for describing the rheology of suspensions: (1) the ‘viscous’ framework in terms of the relative suspension viscosity, η_r , as a function of the reduced solid volume fraction, ϕ_b/ϕ_m , with ϕ_m the maximum flowable packing fraction, and (2) the ‘frictional’ framework in terms of a macroscopic friction coefficient, μ , as a function of the viscous number, I_v , defined as the ratio of the viscous shear stress to the wall-normal particle stress. We focussed on the effect of Coulomb friction between particles, considering three different Coulomb sliding friction coefficients: $\mu_c = 0, 0.2$, and 0.39 , and varied the bulk solid volume fraction from $\phi_b = 0.1$ to 0.6 . We found that η_r scales well with ϕ_b/ϕ_m , with ϕ_m obtained from fitting the Maron-Pierce correlation to the numerical results. We also found that μ scales well with I_v . Furthermore, we found a monotonic relation between ϕ_b/ϕ_m and I_v , which depends only weakly on μ_c . Since $\eta_r = \mu/I_v$, we thus found that the two frameworks are largely equivalent and that both account implicitly for the influence of Coulomb friction on the suspension rheology. However, we found that the normal particle stress differences, N_1 and N_2 , when normalized with the total shear stress and plotted against either ϕ_b/ϕ_m or I_v , remain explicitly dependent on μ_c in a manner that is not yet fully understood.

Third, we simulated pressure-driven flow between two parallel plates to study the effect of heterogeneous shear on the suspension rheology. We varied the bulk solid volume fraction between $\phi_b = 0.2$ and 0.6 , and the Coulomb friction coefficient was set to either $\mu_c = 0$ or 0.5 . The main objectives were to unravel the influence of (1) ϕ_b and μ_c on the flow development time and of (2) heterogeneous shear on the steady-state suspension rheology. Starting from an initially homogeneous distribution, the particles showed shear-induced migration toward the core until equilibrium was reached. The flow development time decays exponentially with increasing ϕ_b/Φ_R , where Φ_R is a friction-dependent reference bulk concentration beyond which particle contacts cause a rapid increase in the particle stress. The steady-state rheology was studied by means of the ‘viscous’ and ‘frictional’ rheology frameworks. Excluding the central core and wall regions, the data for the local relative suspension viscosity collapsed onto a single curve as a function of the normalized local concentration $\bar{\phi}/\phi_m$, where ϕ_m is the friction-dependent maximum flowable packing fraction. The frictional rheology showed ‘subyielding’ at low viscous number I_v in the core region, where the macroscopic friction coefficient μ drops below the minimal value found for homogeneous shear flows. A modified frictional rheology model was presented that captures subyielding. Finally, a model was presented for $\bar{\phi}/\phi_{mp}$ as a function of I_v , where ϕ_{mp} is a modified maximum flowable packing fraction. It captures both ‘overcompaction’ in the core beyond ϕ_m at high ϕ_b and maximum core concentrations below ϕ_m at lower ϕ_b .

Finally, we considered the implications of our findings for printability of dense sus-

pensions in Liquid Deposition Modeling. Utilizing the results from the PR-DNS studies, our approach gives more insight into the fundamental aspects of suspension rheology. However, PR-DNS simulations under these flow conditions are not feasible for day-to-day operations due to the high computational costs and the requirements of computational resources. We identified the important rheological parameters for Liquid Deposition Modeling as the yield stress, the shear-thinning behavior, the viscoelasticity, the thixotropic time, and the stability. We estimated the yield stress from our DNS results and showed that this yield stress can be used in a dimensionless number that shows the printability of suspensions. Furthermore, we described the steps that need to be taken to use our DNS results in regime maps for printability. This is possible using our PR-DNS if the correct flow conditions are implemented, such as oscillatory shear. Additionally, we analysed the extrusion pressure required for 3D printing, and showed that this can be estimated by fitting a Power-law fluid model to the DNS data. This model is capable of accurately capturing the apparent shear-thinning behavior of the suspensions due to particle migration under heterogeneous shear. Lastly, the stability during printing was examined in terms of particle sedimentation in the supply tube of an idle printer. This showed that the sedimentation distance for typical suspensions is limited. However, our results showed that heterogeneity and particle clusters develop at shorter time scales, potentially affecting the suspension rheology when, e.g., printing is resumed after an idle state. Another factor for the stability is shear-induced particle migration, as observed in pressure-driven flow. We showed that, under typical printing conditions, complete migration can happen in tubes as short as 25cm. Moreover, heterogeneity in the particle distribution is already significant at much shorter lengths. The analysis of the results obtained in this work in terms of the printability underlines that a good understanding of the parameters affecting the rheology of dense suspensions is key to develop both equipment and formulations for 3D-printing.

Our findings aid to the understanding of the fundamental suspension dynamics for sedimentation in the strongly confined regime, the effect of solid friction on the suspension rheology, and the difference in rheology for homogeneous and heterogeneous shear flow. Furthermore, we showed that these findings can be used in the application of 3D-printing using the Liquid Deposition Modeling technique, through assessment of the printability.

Samenvatting

Suspensies van vaste deeltjes in een vloeistof komen veel voor in ons dagelijks leven, in de natuur en in de industrie. De industriële toepassing waarop we ons in dit werk richten, is extrusiegebaseerd 3D-printen, waarbij suspensies bijvoorbeeld gebruikt kunnen worden voor het printen van voedsel, metaal of energetische materialen. Voor het printen van energetische materialen moet de belading van de suspensies zo hoog mogelijk zijn om de kwaliteitseisen van het product te behalen. Deze hoge concentratie van vaste deeltjes zorgt ervoor dat de vloeibaarheid van de suspensie omlaag gaat, wat een uitdaging vormt tijdens het printen. Daarnaast kan er verstopping van de printkop ontstaan als deze een vernauwing bevat. Naast de vloeibaarheid speelt de homogeniteit van de suspensie een belangrijke rol, aangezien schuifspanningen en zwaartekracht de neiging hebben om een inhomogene microstructuur te veroorzaken. Bovengenoemde aspecten worden weerspiegeld in de reologie van de suspensie, i.e. de reactie van de suspensie op opgelegde spanning of vervorming. Een goed begrip van de reologie is cruciaal voor het ontwerpen, verbeteren en gebruiken van printsystemen en samenstellingen voor energetische materialen. Het doel van dit onderzoek is om meer inzicht te krijgen in en om de modellering te verbeteren van hoogbeladen suspensies voor het gebruik in UV-assisted Liquid Deposition Modeling.

In het printproces kunnen 4 verschillende fases gedefinieerd worden: (1) stationaire suspensie in het reservoir of de buizen van de printer, (2) stromende suspensie in de toevoerbuis van de printer, (3) suspensie die door de printkop met een contractie stroomt en (4) de uitstroom van de suspensie op het printbed. We hebben particle-resolved Direct Numerical Simulations (PR-DNS) gebruikt om de reologie van suspensies te bestuderen met stromingscondities die fase (1) en (2) van het printproces nabootsen. Met deze simulatietechniek worden de Navier-Stokes vergelijkingen opgelost voor de vloeistof en de Newton-Euler vergelijkingen voor de deeltjes, waarbij we gebruik maken van een frictional soft-sphere collision model voor botsingen tussen deeltjes en van deeltjes met de buiswand. Een rekenkundig efficiënte Immersed Boundary Method is gebruikt voor de koppeling tussen de vloeistof en de deeltjes.

Het eerste deel van deze studie bestond uit simulaties van hoogbeladen viskeuze suspensies die sedimenteren in smalle verticale buizen. Deze stromingsconditie bootst fase (1) van het printproces na. We bestudeerden zowel de sedimentatie van een enkel deeltje als de sedimentatie van suspensies met een bulk volume concentratie (ϕ_b) van 5 tot 30 procent. Het effect van de smalle buis is onderzocht in het bereik met $D/d = 2 - 11$, waarbij D de buisdiameter is en d de deeltjesdiameter. De dynamica van de sedimenterende suspensies is geanalyseerd in termen van onder andere de gemiddelde snelheid en snelheidsfluctuaties, de radiële verdeling van de deeltjes, de dispersie van de deeltjes, en de clustering van deeltjes in de verticale richting. Hiermee hebben we een goed beeld gekregen van het macroscopische gedrag van de suspensie en inzicht in de onderliggende microstructuur. Uit onze analyse bleek dat de gemiddelde sedimentatiesnelheid in smalle

buizen nauwkeurig kan worden beschreven door een aangepaste Richardson-Zaki correlatie waarin de eindsnelheid voor een enkel deeltje dat in de vrije ruimte bezinkt, wordt vervangen door de Francis-correlatie voor sedimentatie in een smalle buis. Voor de verhouding tussen de RMS-waarde en het gemiddelde van de sedimentatiesnelheid vonden we een duidelijke schaling met $\phi_b^{1/3}(D/d)^{2/3}$, met een afwijking van deze schaling voor $D/(d\phi_b^{-1/3}) \lesssim 2.5$. Verder observeerden we, voor $D/d \geq 6$ en $\phi_b = 0.2$, een maximum in de radiale snelheidsverdeling op een afstand van $\approx 1.4d$ van de buiswand, die wijst op een streaming-gedrag waarbij langwerpige dichte deeltjesclusters sneller sedimenteren dan de omringende, meer verdunde gebieden. We concludeerden dat de dynamica van de sedimenterende suspensie in het bestudeerde regime sterk wordt beïnvloed door de smalle buis, met een verandering in schalingsgedrag bij $D/(d\phi_b^{-1/3}) \lesssim 2.5$ en $D/d \lesssim 4$.

In het tweede deel van dit werk hebben we de reologie van suspensies in een afschuifstroming bestudeerd om een beter inzicht te krijgen in de modellering van de suspensiereologie voor fase (2) van het printproces. We hebben twee veelgebruikte beschrijvingen voor de reologie van suspensies vergeleken: (1) de viskeuze beschrijving die de reologie uitdrukt in termen van de viscositeit als functie van de genormaliseerde volume fractie (ϕ_b/ϕ_m) waarbij ϕ_m de maximale volume fractie is waarbij de suspensie nog vloeibaar is, en (2) de beschrijving gebaseerd op wrijving die de reologie uitdrukt in termen van de macroscopische wrijvingscoëfficiënt (μ) als functie van het viskeuze getal (I_v) dat is gedefinieerd als de verhouding tussen de viskeuze schuifspanning en de wandnormale deeltjesspanning. De focus lag hierbij op het effect van wrijving tussen deeltjes met drie verschillende Coulomb wrijvingscoëfficiënten: $\mu_c = 0, 0.2$, en 0.39 . Daarnaast hebben we de concentratie van deeltjes gevarieerd over een bereik van $\phi_b = 0.1$ tot 0.6 . We ontdekten dat de relatieve viscositeit (η_r) goed schaalt met ϕ_b/ϕ_m , waarbij ϕ_m is verkregen door de Maron-Pierce correlatie te fitten aan de DNS data. We stelden ook vast dat μ schaalt met I_v . Verder observeerden we een monotoon verband tussen ϕ_b/ϕ_m en I_v dat slechts zwak afhankelijk is van de Coulomb wrijvingscoëfficiënt. Aangezien $\eta_r = \mu/I_v$, concludeerden we dat de twee beschrijvingen grotendeels equivalent zijn en dat beide impliciet rekening houden met Coulomb-wrijving. We constateerden echter dat de normaalspanningsverschillen, N_1 en N_2 , wanneer genormaliseerd met de totale schuifspanning en uitgezet tegen ϕ_b/ϕ_m of I_v , expliciet afhankelijk blijven van μ_c op een manier die nog niet volledig begrepen is.

Het derde deel van deze studie bestond uit simulaties van drukgedreven stroming tussen twee vlakke platen om het effect van heterogene afschuiving op de reologie van de suspensie te bestuderen. We varieerden de volumefractie van de vaste stof tussen $\phi_b = 0.2$ en 0.6 , en de Coulomb-wrijvingscoëfficiënt werd ingesteld op $\mu_c = 0$ of 0.5 . De belangrijkste doelstellingen waren het ontrafelen van de invloed van (1) ϕ_b en μ_c op de ontwikkelingstijd van de stroming en van (2) heterogene schuifspanning op de reologie van de suspensie voor een volledig ontwikkelde stroming. Uitgaande van een aanvankelijk homogene verdeling vertoonden de deeltjes schuifspannings-geïnduceerde migratie naar het midden van het kanaal totdat evenwicht werd bereikt. De ontwikkelingstijd van de stroming neemt exponentieel af met toenemende ϕ_b/Φ_R , waarbij Φ_R een wrijvingsafhankelijke referentieconcentratie is waarboven deeltjescontacten een snelle toename van de deeltjesspanning veroorzaken. De reologie voor een volledig ontwikkelde stroming werd bestudeerd met behulp van de ‘viskeuze’ en ‘wrijvings’ beschrijvingen van de reologie. Met uitzondering van de kern- en wand-gebieden vallen de gegevens voor de lokale relatieve suspensievis-

cositeit samen op één enkele curve als functie van de genormaliseerde lokale concentratie ($\bar{\phi}/\phi_m$). De wrijvingsreologie vertoonde ‘subvloeien’ bij een laag viskeus getal in het kerngebied, waar de macroscopische wrijvingscoëfficiënt onder de minimale waarde daalt die gevonden wordt voor homogene schuifstroming. We presenteerden een aangepast wrijvingsreologiemodel dat subvloeien beschrijft. Ten slotte presenteerden we een model voor $\bar{\phi}/\phi_{mp}$ als functie van I_v , waarbij ϕ_{mp} een aangepaste maximale vloeibare concentratie is. Het model beschrijft zowel ‘overcompactie’ in de kern voorbij ϕ_m bij hoge ϕ_b als maximale kernconcentraties onder ϕ_m bij lagere ϕ_b .

Ten slotte hebben we de implicaties van onze bevindingen voor de printbaarheid van hoogbeladen suspensies in Liquid Deposition Modeling (LDM) overwogen. Onze aanpak met behulp van directe numerieke simulaties geeft meer inzicht in de fundamentele aspecten van de reologie van suspensies. PR-DNS-simulaties onder deze stromingscondities zijn echter niet bruikbaar voor dagelijkse werkzaamheden door de grote rekenkracht die vereist is om zulke simulaties uit te voeren. We hebben de belangrijke reologische parameters voor Liquid Deposition Modeling geïdentificeerd als de vloeigrens, het schuifverdunningsgedrag, de visco-elasticiteit, de thixotrope tijd en de stabiliteit. We hebben de vloeigrens afgeschat op basis van onze DNS-resultaten en laten zien dat deze vloeigrens kan worden gebruikt in een dimensieloos getal dat de printbaarheid van suspensies beschrijft. Verder beschreven we de stappen die nodig zijn om onze DNS-resultaten te gebruiken in regimekaarten voor printbaarheid. Dit is mogelijk met onze PR-DNS als de juiste stromingscondities worden geïmplementeerd, zoals oscillerende schuifspanning. Daarnaast hebben we de extrusiedruk in beschouwing genomen en aangetoond dat deze kan worden beschreven door een Power-law vloeistofmodel aan de DNS-gegevens te fitten. Dit model is in staat de schijnbare schuifverdunding van de suspensies, veroorzaakt door deeltjesmigratie onder invloed van heterogene afschuiving, nauwkeurig te beschrijven. Ten slotte werd de stabiliteit tijdens het printen onderzocht in termen van deeltjes sedimentatie in de toevoerbuizen van een stilstaande printer. Dit toont aan dat de sedimentatieafstand voor typische suspensies beperkt is, maar onze resultaten laten zien dat heterogeniteit en deeltjesclusters zich ontwikkelen op kortere tijdschalen. Een andere factor in de stabiliteit is schuifspannings-geïnduceerde deeltjesmigratie, zoals waargenomen in drukgedreven stroming. We hebben aangetoond dat onder typische printomstandigheden volledige migratie kan plaatsvinden in buizen met een lengte van slechts 25 cm. Bovendien is de heterogeniteit in de deeltjesverdeling al significant bij veel kortere lengtes. De analyse van de in dit werk verkregen resultaten met betrekking tot de printbaarheid onderstreept dat een goed begrip van de reologie van suspensies essentieel is voor de ontwikkeling van zowel apparatuur als formuleringen voor 3D-printen.

Onze bevindingen dragen bij aan het begrip van de fundamentele suspensiedynamiek voor sedimentatie in smalle buizen, het effect van wrijving tussen deeltjes op de reologie van de suspensie en het verschil in reologie voor homogene en heterogene schuifstroming. Daarnaast hebben we aangetoond dat deze bevindingen kunnen worden gebruikt bij de toepassing van 3D-printen met behulp van de Liquid Deposition Modeling-techniek door de printbaarheid te beoordelen.

1

Introduction

In this chapter we introduce the use of suspensions in 3D-printing applications and define the type of suspensions that we study in this work. The literature is reviewed to highlight the importance of the rheology for this application. Furthermore, we look at the factors that affect the rheology of suspensions and how these factors are included in the description of the rheology. From this literature review we identify the gaps and define the research questions that we want to answer in this work.

1

If we look around us, we can find numerous examples of solid particles dispersed in a liquid. Solid-liquid suspensions are commonly encountered in daily life, in our house we can find them as, for example: solid particles in toothpaste, fruit pieces in yoghurt, and pigments in paint. In our environment, these suspensions appear as sediment in rivers, fresh concrete for construction projects, and solid waste in sewer systems. Next to that, suspensions play an important role in many industrial processes, such as dredging, food processing, and chemical reactors. Some of these examples are shown in Figure 1.1.



(a)



(b)



(c)



(d)

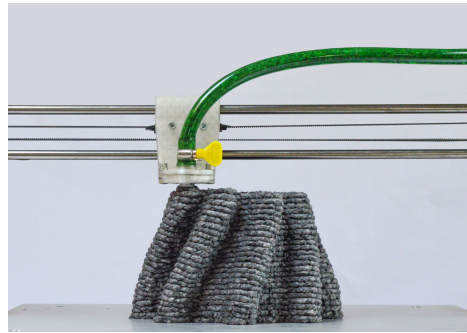
Figure 1.1: Examples of solid-liquid suspensions in our daily life, in the environment, and in industry: (a) fruit pieces and seeds in yoghurt [1], (b) sediment discharge from a river into the sea [2], (c) pouring of fresh concrete for construction work [3], and (d) spraying of a sand/water mixture for land reclamation [4].

These examples span a wide range of length and timescales, and the properties of the suspensions vary tremendously. If we consider dredging and sediment transport, the density ratio is usually large and the flow rates are typically high, leading to turbulent conditions. In contrast, cosmetic products usually need to be stable over a long period of time, requiring a small density ratio or a high viscosity carrier fluid to avoid sedimentation. To be able to design, produce, and transport these suspensions while maintaining the desired properties, a thorough understanding of the suspension rheology is required, i.e., the behavior of the suspension under imposed flow conditions.

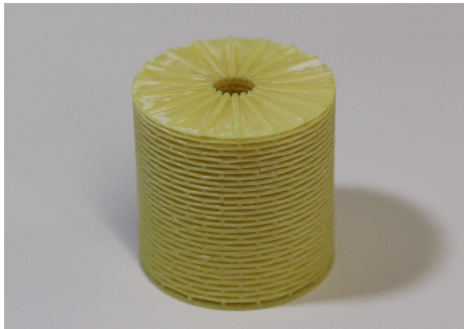
The imposed flow conditions that we consider in this work are those of an application that is not typically associated with suspensions, namely 3D-printing. In 3D-printing, suspensions can be used to improve the material properties or to add functionality to otherwise simple materials, and even to enable printing with new materials [5]. Improving material properties can be done by adding fillers to a matrix to enhance the mechanical strength, as is done with glass- or carbon fiber in polymer matrices [6]. Adding functionality to 3D-prints can be done for instance by adding conductive particles to the polymer, such as carbon nanotubes or ceramic particles. If these filled materials are then printed at specific locations during the printing process, conductive paths can be created in a product [7]. Examples of printing with new materials, such as paper pulp and energetic materials, are shown in Figure 1.2.



(a)



(b)



(c)



(d)

Figure 1.2: Examples of printing methods that utilize suspensions as a printing material: (a) pasta dough [8], (b) paper pulp [9], (c) energetic materials [10], and (d) metal [11].

Different additive manufacturing techniques have their own advantages and limitations when they are used in combination with suspensions. For example, in Stereolithography (SLA), a printing method in which a UV laser is used to cure layers of liquid photopolymer resin in a vat, the solid volume fraction can not be too high as the material needs to flow into a narrow gap between the previous layer and the build platform. Fused Deposition Modelling (FDM) with suspensions requires composite filaments, which al-

ready contain the filler, that are heated in order to flow and fuse together on a print bed. Challenges in printing with composite filaments are for example that the filament melting behavior is influenced by the filler, or that hard fillers cause more wear on the equipment due to their abrasiveness [6]. A method that is more compatible with dense suspensions is Direct Ink Writing (DIW) or Liquid Deposition Modelling (LDM), where a fluid-like material is extruded onto the print bed after which it transitions to a solid state. This transition can happen by several different mechanisms, for example: solvent evaporation [12, 13], gelation [14], uv-curing [12, 13, 15], or heat-curing [16].

The printing application of interest in this work is used to print energetic materials (such as propellants, explosives, or pyrotechnics), which are generally unstable at high temperatures as used in FDM. Performance requirements of energetic materials dictate that the solid content should be as high as possible. This high solid load creates a challenge to maintain flowable conditions. Additionally, this high volume fraction can create problems with blocking of the nozzle if a contraction is used at the end. Next to the flowability, the homogeneity of the suspension plays an important role, where shear stresses and gravity tend to cause inhomogeneous microstructures. The desire to print gradients in solid content, accompanied by rapid changes in suspension properties and flow conditions, poses an additional challenge. To solve these technical challenges, TNO (Netherlands Organization for Applied Scientific Research) has developed a new 3D-printer to print energetic materials at high solid loads [17]. The technique used in this printer can be best described by UV-assisted Liquid Deposition Modelling (UV-LDM), in which a highly filled UV-curing resin is extruded through the printing nozzle where it is illuminated by a UV light to start the photopolymerization. In this printing method, the viscosity, yield stress, and shear modulus affect the print quality [13, 15]. These parameters are captured by the rheology of the material, making it very important to understand the rheology of dense suspensions. When changing compositions or materials, a solid understanding of the rheology can help guide choices and adjustment of printing parameters. It may even be possible to change the properties of the suspension components to reach a certain desired rheology that is needed for the printing application. Although the rheology (or fluid mechanics) is an important aspect in the printing process, the chemistry and solid mechanics should not be overlooked. These aspects play a role in the curing behavior of the polymer matrix after extrusion and in the mechanical properties of the printed product, respectively. The current work was part of a larger program, where one PhD project focussed on the solid mechanics and stability of 3D-printed energetic materials, whereas the current project focussed on the fluid mechanics aspect of the printing application. More specifically, this work focussed on the challenges related to the flowability and homogeneity at high packing fractions. In other words, the rheology of dense suspensions.

Before we can discuss the current understanding of suspension rheology, we first need to distinguish which kind of suspensions we consider. Therefore, we first outline the different types of suspensions. Suspensions are typically categorized by a number of criteria. The first distinction we make is by particle size [18]. Suspensions with small particles ($d \leq 1\mu\text{m}$) are classified as colloidal, whereas suspensions with larger particles ($d \geq 5\mu\text{m}$) are classified as non-colloidal. This classification is often expressed using the Péclet number (Pe), defined as the ratio of advective transport by (shear) flow and diffusive transport

by Brownian motion. Therefore, the Péclet number is a function of the particle diameter (d), the fluid viscosity (η_0), the temperature (T), and the shear rate ($\dot{\gamma}$): $Pe = 3\pi\eta_0\dot{\gamma}d^3/(k_B T)$ with k_B the Boltzmann constant. The second distinction can be made based on the carrier fluid being Newtonian or non-Newtonian. For Newtonian carrier fluids, the suspensions will exhibit Newtonian rheology at low solid volume fractions and non-Newtonian rheology will come into play at increasing solid volume fractions due to hydrodynamic and contact interactions between particles. In contrast, non-Newtonian carrier fluids interact differently with particles depending on their properties, typically the addition of particles enhances the non-Newtonian characteristics of the fluid [19]. Third, the particle shape and size distribution affect the particle-fluid and particle-particle interactions. The particle shape affects the microstructure of the suspension, which in turn has a strong influence on the rheology [20]. Particle size distribution also affects the rheology. A broader particle size distribution typically leads to a lower viscosity at constant solid volume fraction [21], and shifts the onset of shear-thickening to higher values of critical shear rates due to changes in particle interactions [22]. Finally, the density difference of the solid and the fluid phase, $\rho_p - \rho_f$, influences the tendency for the particles to settle down (or float) under the action of gravity. The sedimentation dynamics of a single particle are governed primarily by the Galileo number (Ga), defined as the particle Reynolds number based on the particle diameter and the inertio-gravitational velocity scale [23], and scales with the square root of the particle-fluid density difference: $Ga = \sqrt{(\rho_p - \rho_f)gd^3/(\rho_f\eta_0)}$. For $Ga \gtrsim 155$, which corresponds to the inertial flow regime, the sedimentation dynamics are also directly influenced by the particle-fluid density ratio; for the same Ga value, the settling path and wake structure of the particle may be very different dependent on the density ratio [23]. In this work, we consider *non-colloidal* suspensions, for which $Pe \gg 1$, in a *Newtonian* carrier fluid with *spherical* particles that are *monodisperse* in size. The density ratio is either set to 1 (i.e., neutrally-buoyant particles with $Ga = 0$) in our rheology studies or set to 1.05 (typical for plastic particles in water) in our sedimentation study (with $Ga = \sqrt{18}$), as described in more detail below.

The rheology of such suspensions has been studied extensively for many years since pioneering work by Albert Einstein [24, 25], who introduced a relation for the relative shear viscosity of a dilute suspension of spheres as a function of the solid volume fraction. A good overview of the subject is given in several review articles [19, 26, 27]. Relative to the viscosity of the carrier fluid, η_0 , suspensions show an increase in shear mixture viscosity, η , for increasing bulk solid volume fraction, ϕ_b . Typically, three different regimes are distinguished, dependent on the bulk solid volume fraction: the dilute regime for $\phi_b \lesssim 0.05$, the semi-dilute regime for $0.05 \lesssim \phi_b \lesssim 0.2$, and the dense regime for $\phi_b \gtrsim 0.2$. In the dilute regime, the particles only interact with the fluid matrix, while not interacting with each other. The relative viscosity, η/η_0 , for this regime was theoretically derived by Einstein [24, 25]: $\eta/\eta_0 = 1 + (5/2)\phi_b$. This theoretical relation was later expanded to include second-order interactions by Batchelor and Green [28], which describes the relative viscosity up to the semi-dilute regime. In the dense regime, the particle interactions become increasingly important and particle contacts come into play. For this regime, theoretical relations are not feasible anymore due to the many-body interactions, forcing the community to revert to empirical correlations to describe the suspension viscosity [29, 30, 31]. These relations

show that close to the jamming limit, $\phi_b \rightarrow \phi_m$ with ϕ_m the maximum flowable packing fraction, the relative viscosity can be accurately modelled as a function of ϕ_b/ϕ_m (or, alternatively, as a function of $\phi_m - \phi_b$ [32]). Figure 1.3 shows the relations mentioned above, experimental data [33, 34], and numerical results [35, 36, 37, 38, 39, 40] from literature for simple (i.e., homogeneous) shear flows of a homogeneous suspension.

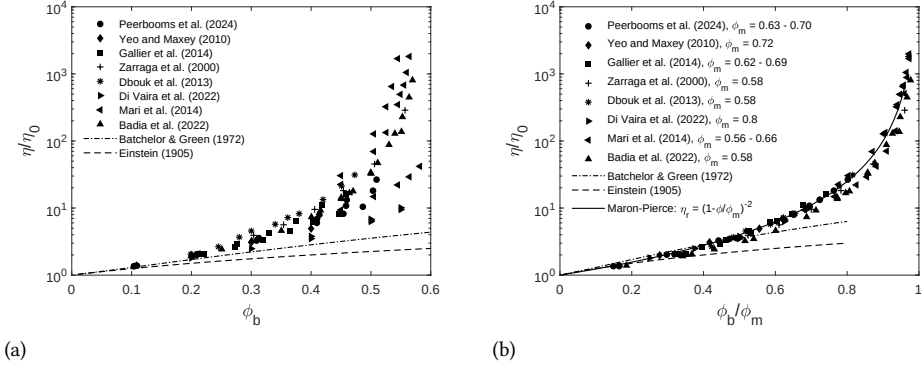


Figure 1.3: Relative shear viscosity of a homogeneous suspension in simple shear flow as a function of the (a) bulk solid volume fraction, and (b) the normalized bulk solid volume fraction. Data is compiled from various experimental [33, 34] and numerical [35, 36, 37, 38, 39, 40] studies in literature.

This shows that the relative viscosity can be scaled for a large variety of suspension compositions with different carrier fluids and particles characteristics. However, for all these conditions ϕ_m is different and depends on the properties of the suspension. Therefore, in the dense regime, the particle characteristics, such as shape, roughness, and size distribution, are very important. Literature shows that the maximum flowable packing fraction depends on the particle size distribution [41, 21] and the interparticle friction coefficient [37, 38, 42]. A remaining question is, however, which particle characteristics are accounted for in ϕ_m , and if this scaling extends beyond the shear viscosity to, for instance, normal stresses.

The suspension shear viscosity does not provide a complete description of the suspension rheology as dense suspensions can also exhibit shear-rate dependent behavior such as yield stresses [43], shear thinning [18, 44], and (dis)continuous shear thickening [45, 38, 46, 47]. Furthermore, normal stress differences are observed for dense suspensions [19]. The origin of normal stress differences lies in the microstructure of the suspension, i.e. the spatial distribution of particles in the carrier fluid. The resulting normal stress differences, $N_1 = \Sigma_{11} - \Sigma_{22}$ and $N_2 = \Sigma_{22} - \Sigma_{33}$, are not completely understood and there is no clear consensus in literature about the sign and magnitude. The lack of consensus also leads to inconsistency in models to describe the normal stress differences. Figure 1.4 shows the normal stress differences compiled from various experimental [33, 34] and numerical [35, 37, 40, 48] studies in literature. The spread of the data shown in this figure illustrates that more work needs to be done to understand the normal stress differences in order to improve constitutive modelling.

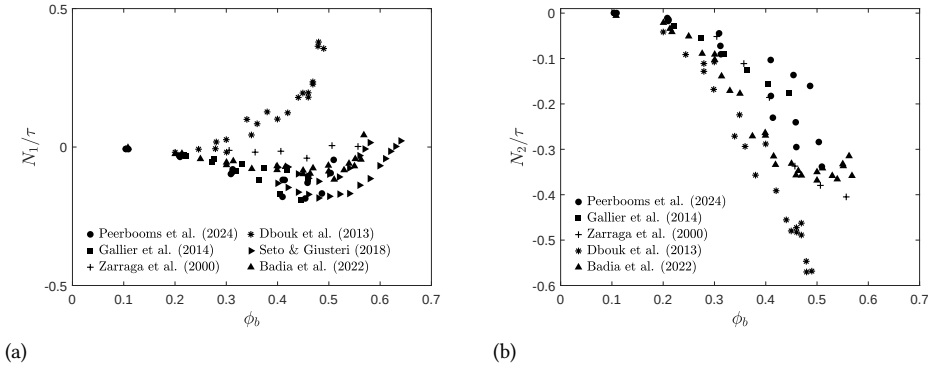


Figure 1.4: Normal stress differences of a homogeneous suspension in simple shear flow (a) N_1 and (b) N_2 , both normalized by the total shear stress (τ , the sum of the viscous and the particle shear stress), and shown as a function of the solid volume fraction. Data is compiled from various experimental [33, 34] and numerical [35, 37, 40, 48] studies in literature.

An alternative description to the *viscous* rheology framework, which describes the rheology in terms of the suspension viscosity, is the *frictional* rheology framework introduced by Boyer et al. [32]. Herein, the rheology is described as a function of the viscous number, I_v , which effectively captures the ratio of the viscous shear stress and particle pressure, which is crucial for describing the rheology of these systems. The resistance to flow is described using the macroscopic friction coefficient, $\mu(I_v)$, which is defined as the ratio of the total shear stress, τ , to the particle pressure. This frictional rheology description has shown to work well for homogeneous shear flows; however, the application of the framework to inhomogeneous shear flows, such as pressure-driven flow, has only recently received more attention [49, 42]. One of the main challenges in extending the framework is how to account for non-local phenomena such as subyielding (i.e., a vanishing shear stress at a finite local normal stress) and overcompaction (i.e., a local packing fraction exceeding the maximum possible value in simple, homogeneous, shear flows) [50, 51]. Nevertheless, being able to describe the rheology of dense suspensions in non-homogeneous shear flows is of great importance to be able to tackle real-life flow conditions (such as encountered in 3D-printing) where inhomogeneous shear is often encountered.

The discussion above highlights that the microstructure is very important for the suspension rheology, influencing for instance the viscosity and normal stresses. In turn, the microstructure depends on the solid volume fraction, particle properties, and flow conditions. Under homogeneous shear conditions, suspended particles do not show a collective net displacement. While this can be the case for inhomogeneous shear conditions, such as oscillatory flow, or pressure-driven flow. In pressure-driven tube flow, for which the flow experiences varying shear dependent on the radial position, the particles tend to migrate resulting in an inhomogeneous concentration distribution (even if the initial distribution was homogeneous). For dense suspensions at low Reynolds numbers, shear-induced migration resulting from particle-particle interactions causes the particles to move to low-

shear zones until an equilibrium is reached. This means that the particles move towards the centerline of the tube [52, 53], which is often described using the suspension balance model (SBM) [54, 55, 56]. At higher Reynolds numbers, inertial effects may induce lift forces resulting in migration such as the tubular pinching effect related to particle-fluid interactions. For increasing concentration, this is overwhelmed by shear-induced migration from particle-particle interactions [57]. The latter may be augmented by inertia, dubbed as inertial shear thickening by Picano et al. [58, 59].

The microstructure is also affected by the tendency of particles to settle under the influence of gravity. The effect of solid volume fraction on the sedimentation velocity has been studied extensively, where for dense suspensions hindered settling plays an important role [60, 61]. The mean sedimentation velocity can be described by empirical correlations for hindered settling [60, 61, 62, 63]. Furthermore, in the tubes of a 3D-printer, which may be narrow when compared to the largest particle diameter in the suspension, the effect of confinement needs to be taken into account. The effect of confinement has been studied over a wide range of confinement ratios, $\lambda = d/D$ with D the tube diameter, and Reynolds numbers, leading to correlations that take confinement into account for the sedimentation velocity [64, 65, 66, 67, 68, 69, 61]. However, for dense suspensions in narrow vertical tubes, the dynamics are not fully understood yet. Moreover, the effect of sedimentation on particle velocity fluctuations, and the inherent effect on the microstructure, have long been topic of discussion [70, 71, 72, 73, 74, 75]. More research is needed to understand how these factors affect 3D-printing of dense suspensions.

The **goal** of this research is to gain more insight into and to improve modeling of the rheology of dense suspensions for the application in UV-assisted Liquid Deposition Modelling. Therefore, we identified multiple stages in the printing process: (1) stationary suspension in the reservoir and tubes of the printer, (2) suspension flowing through the supply tube of the printer, (3) suspension flowing through the nozzle, and (4) suspension deposited on the printing platform. In this work we focus on stages (1) and (2), that pertain to the flow behavior and rheology of dense suspensions. The main research questions that we want to answer are:

1. **What is the effect of the tube-to-particle diameter ratio on the sedimentation dynamics in a viscous fluid?**

The stability of suspensions is a concern in 3D-printing, as settling of particles can create inhomogeneous distributions when the printer is idle. Therefore, we focus on the effect of tube-to-particle diameter ratio in narrow vertical tubes. The dynamics are considered in terms of the mean sedimentation velocity, velocity fluctuations, and suspension microstructure.

2. **How does solid (interparticle) friction affect the rheology in simple shear flow?**

Rheology is often studied under well-controlled flow conditions, of which simple shear flow is common in experimental and numerical studies. To get a better understanding of the suspension rheology we study the effect of the interparticle friction coefficient. Common frameworks that are used in the literature to describe the rhe-

ology of dense suspensions are compared to answer the question: **Are the viscous and frictional rheology frameworks fully equivalent?**

3. How does the suspension rheology under heterogeneous shear differ from the suspension rheology under homogeneous shear conditions?

The flow in the tubes of an LDM 3D-printer is typically forced by a moving piston or an applied pressure difference. This flow condition results in an applied heterogeneous shear rate. We varied the solid volume concentration and the interparticle friction coefficient to investigate the scaling of the rheology under these conditions. As discussed above, particles migrate under the applied flow conditions leading to the question: **How do these parameters affect particle migration?** Additionally, we study the steady-state rheology where we are interested in: **Can the frictional rheology framework developed for simple (homogeneous) shear flows be extended to pressure-driven flow?**

We employ particle-resolved Direct Numerical Simulations (PR-DNS) to study the suspension rheology under conditions that allow us to answer these questions. In the PR-DNS, the full Navier-Stokes equations are solved for the fluid phase, combined with the Newton-Euler equations for the motion of the particles, including a frictional soft-sphere collision model for particle collisions/contacts [76, 57]. A computationally efficient Immersed Boundary Method is employed for the fluid-solid coupling [77, 78]. In our first study, we consider the sedimentation of dense suspensions in narrow vertical tubes. In our second study, we consider simple shear between two parallel plates. In our third study, we consider pressure-driven flow between two parallel plates. These conditions are schematically illustrated in Figure 1.5. For all these conditions, we use spherical particles of a single diameter at slow flow conditions, resembling a viscous carrier fluid. We vary the solid volume concentration and the interparticle friction coefficient to assess the effect on the suspension rheology. The results are analyzed in terms of velocity profiles, concentration profiles, microstructure, and stress contributions, among others. These properties are then used for modelling of the rheology of dense suspensions. Modelling of the rheology of dense suspensions is important to be able to predict the properties and therewith the printability of compositions.

The results are presented and discussed in the following chapters, which are structured as follows. In Chapter 2, the sedimentation of dense suspensions in narrow vertical tubes is discussed. In Chapter 3, the rheology of the suspension is discussed based on simulations done in plane Couette flow conditions. In Chapter 4, the particle migration and rheology are discussed for pressure-driven channel flow. Chapter 5 outlines how the results of our research can be used to improve and optimize 3D-printing of dense suspensions by LDM. And to conclude, Chapter 6 contains the conclusions we draw from our research and the recommendations for future work.

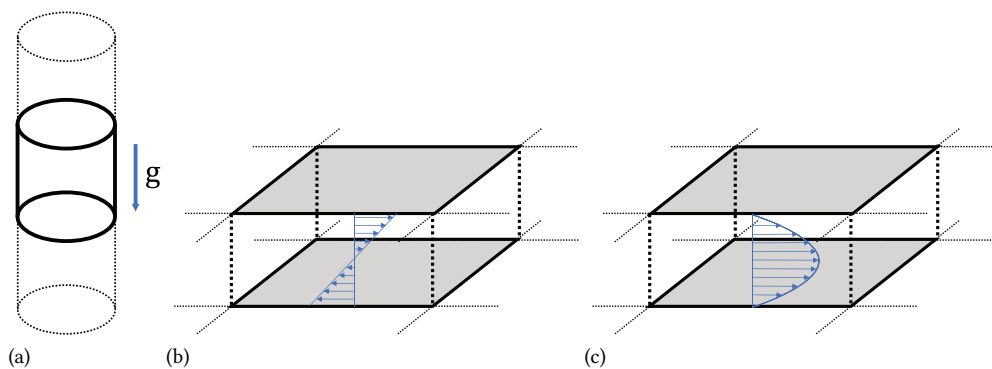


Figure 1.5: Schematic representation of the three conditions used to investigate the rheology of dense suspensions: (a) sedimentation in narrow vertical tubes, (b) plane Couette flow, and (c) pressure-driven plane channel flow.

References

- [1] Image of fruit pieces and seeds in yoghurt. online, <https://pixabay.com/photos/yogurt-chia-seeds-fruits-strawberry-1235353/>, accessed 06 June 2025.
- [2] Image of a sediment plume at sea. online, https://www.esa.int/ESA_Multimedia/Images/2019/02/Sediment_plume_at_sea, accessed 14 January 2025. Contains modified Copernicus Sentinel data (2019), processed by ESA, image was cropped from the original.
- [3] Image of pouring of fresh concrete for construction work. online, <https://www.vecteezy.com/photo/19927055-pouring-cement-during-for-construction>, accessed 06 June 2025.
- [4] Image of spraying of a sand/water mixture for land reclamation. online, <https://pixabay.com/photos/dredging-nourishment-beach-sand-2955269/>, accessed 06 June 2025.
- [5] Nurhalida Shahrubudin, Te Chuan Lee, and RJPM Ramlan. An overview on 3d printing technology: Technological, materials, and applications. *Procedia manufacturing*, 35:1286–1296, 2019.
- [6] Antreas Kantaros, Evangelos Soulis, Florian Ion Tiberiu Petrescu, and Theodore Ganetsos. Advanced composite materials utilized in fdm/fff 3d printing manufacturing processes: the case of filled filaments. *Materials*, 16(18):6210, 2023.
- [7] Hyunwoo Yuk, Baoyang Lu, Shen Lin, Kai Qu, Jingkun Xu, Jianhong Luo, and Xuanhe Zhao. 3d printing of conducting polymers. *Nature communications*, 11(1):1604, 2020.
- [8] Image of 3d-printing of pasta dough. online, <https://3dprint.com/151348/barilla-pasta-3d-printer/>, accessed 18 June 2025.
- [9] Image of 3d-printing of paper pulp. online, <https://materialdistrict.com/article/paper-pulp-printer/>, accessed 18 June 2025.
- [10] Photo courtesy of TNO. Image of 3d-printed part comprising energetic material.
- [11] Image of 3d-printed metal parts. online, <https://www.pim-international.com/articles/metal-additive-manufacturing-micro-parts-how-computational-engineering-methods-can-enable-new-micro-robotic-applications/>, accessed 18 June 2025. image was cropped from the original.
- [12] Jackson K Wilt, Dustin Gilmer, Sungjin Kim, Brett G Compton, and Tomonori Saito. Direct ink writing techniques for in situ gelation and solidification. *MRS Communications*, 11:106–121, 2021.

- [13] Alexandra Marnot, Katie Koube, Sungwoo Jang, Naresh Thadhani, Josh Kacher, and Blair Brettmann. Material extrusion additive manufacturing of high particle loaded suspensions: a review of materials, processes and challenges. *Virtual and Physical Prototyping*, 18(1):e2279149, 2023.
- [14] Amin M'barki, Lydéric Bocquet, and Adam Stevenson. Linking rheology and printability for dense and strong ceramics by direct ink writing. *Scientific reports*, 7(1):6017, 2017.
- [15] John P Reynolds, Daniel A Rau, Christopher B Williams, and Michael J Bortner. A rheological method to predict printability of high solids content inks via ultraviolet-assisted material extrusion. *Additive Manufacturing*, 75:103753, 2023.
- [16] Chongjie Gao, Jingjing Qiu, and Shiren Wang. In-situ curing of 3d printed freestanding thermosets. *Journal of Advanced Manufacturing and Processing*, 4(3):e10114, 2022.
- [17] Joost van Lingen. Gradient additive manufacturing of energetics research (gamer). *Netherlands Organisation for Applied Scientific Research*, 2022.
- [18] BM Guy, Michiel Hermes, and Wilson CK Poon. Towards a unified description of the rheology of hard-particle suspensions. *Physical review letters*, 115(8):088304, 2015.
- [19] Élisabeth Guazzelli and Olivier Pouliquen. Rheology of dense granular suspensions. *Journal of Fluid Mechanics*, 852, 2018.
- [20] M Mahmoudian, F Goharpey, M Behzadnasab, and Z Daneshfar. Shear thickening and hysteresis in dense suspensions: The effect of particle shape. *Journal of Rheology*, 68(3):479–490, 2024.
- [21] Sidhant Pednekar, Jaehun Chun, and Jeffrey F Morris. Bidisperse and polydisperse suspension rheology at large solid fraction. *Journal of Rheology*, 62(2):513–526, 2018.
- [22] T Ajeeth Prabhu and Anugrah Singh. Effect of carrier fluid and particle size distribution on the rheology of shear thickening suspensions. *Rheologica Acta*, 60:107–118, 2021.
- [23] Shravan KR Raaghav, Christian Poelma, and Wim-Paul Breugem. Path instabilities of a freely rising or falling sphere. *International Journal of Multiphase Flow*, 153:104111, 2022.
- [24] Albert Einstein. *Eine neue Bestimmung der Moleküldimensionen*. PhD thesis, ETH Zurich, 1905.
- [25] Albert Einstein. Berichtigung zu meiner arbeit: Eine neue bestimmung der moleküldimensionen. *Annalen der Physik*, 339(3):591–592, 1911.
- [26] Jonathan J Stickel and Robert L Powell. Fluid mechanics and rheology of dense suspensions. *Annu. Rev. Fluid Mech.*, 37:129–149, 2005.
- [27] Christopher Ness, Ryohei Seto, and Romain Mari. The physics of dense suspensions. *Annual Review of Condensed Matter Physics*, 13:97–117, 2022.

- [28] GK Batchelor and JT Green. The determination of the bulk stress in a suspension of spherical particles to order c^2 . *Journal of Fluid Mechanics*, 56(3):401–427, 1972.
- [29] H Eilers. Die viskosität von emulsionen hochviskoser stoffe als funktion der konzentration. *Kolloid-Zeitschrift*, 97(3):313–321, 1941.
- [30] Samuel H Maron and Percy E Pierce. Application of ree-eyring generalized flow theory to suspensions of spherical particles. *Journal of colloid science*, 11(1):80–95, 1956.
- [31] Irvin M Krieger and Thomas J Dougherty. A mechanism for non-newtonian flow in suspensions of rigid spheres. *Transactions of the Society of Rheology*, 3(1):137–152, 1959.
- [32] François Boyer, Élisabeth Guazzelli, and Olivier Pouliquen. Unifying suspension and granular rheology. *Physical review letters*, 107(18):188301, 2011.
- [33] Isidro E Zarraga, Davide A Hill, and David T Leighton Jr. The characterization of the total stress of concentrated suspensions of noncolloidal spheres in newtonian fluids. *Journal of Rheology*, 44(2):185–220, 2000.
- [34] Talib Dbouk, Laurent Lobry, and Elisabeth Lemaire. Normal stresses in concentrated non-brownian suspensions. *Journal of Fluid Mechanics*, 715:239–272, 2013.
- [35] Wouter Peerbooms, Tim Nadorp, Antoine van der Heijden, and Wim-Paul Breugem. Interparticle friction in sheared dense suspensions: Comparison of the viscous and frictional rheology descriptions. *Journal of Rheology*, 68(2):263–283, 2024.
- [36] Kyongmin Yeo and Martin R Maxey. Numerical simulations of concentrated suspensions of monodisperse particles in a poiseuille flow. *Journal of fluid mechanics*, 682:491–518, 2011.
- [37] Stany Gallier, Elisabeth Lemaire, François Peters, and Laurent Lobry. Rheology of sheared suspensions of rough frictional particles. *Journal of Fluid Mechanics*, 757:514–549, 2014.
- [38] Romain Mari, Ryohei Seto, Jeffrey F Morris, and Morton M Denn. Shear thickening, frictionless and frictional rheologies in non-brownian suspensions. *Journal of Rheology*, 58(6):1693–1724, 2014.
- [39] Nathan J Di Vaira, Łukasz Łaniewski-Wołk, Raymond L Johnson, Saiied M Aminossadati, and Christopher R Leonardi. Influence of particle polydispersity on bulk migration and size segregation in channel flows. *Journal of Fluid Mechanics*, 939:A30, 2022.
- [40] Ayoub Badia, Yves D’Angelo, François Peters, and Laurent Lobry. Frame-invariant modeling for non-brownian suspension flows. *Journal of Non-Newtonian Fluid Mechanics*, 309:104904, 2022.

- [41] Kenneth W Desmond and Eric R Weeks. Influence of particle size distribution on random close packing of spheres. *Physical Review E*, 90(2):022204, 2014.
- [42] William Chèvremont, Bruno Chareyre, and Hugues Bodiguel. Quantitative study of the rheology of frictional suspensions: Influence of friction coefficient in a large range of viscous numbers. *Physical Review Fluids*, 4(6):064302, 2019.
- [43] Abhinendra Singh, Sidhant Pednekar, Jaehun Chun, Morton M Denn, and Jeffrey F Morris. From yielding to shear jamming in a cohesive frictional suspension. *Physical review letters*, 122(9):098004, 2019.
- [44] Laurent Lobry, Elisabeth Lemaire, Frédéric Blanc, Stany Gallier, and François Peters. Shear thinning in non-brownian suspensions explained by variable friction between particles. *Journal of Fluid Mechanics*, 860:682–710, 2019.
- [45] Ryohei Seto, Romain Mari, Jeffrey F Morris, and Morton M Denn. Discontinuous shear thickening of frictional hard-sphere suspensions. *Physical review letters*, 111(21):218301, 2013.
- [46] Abhinendra Singh, Romain Mari, Morton M Denn, and Jeffrey F Morris. A constitutive model for simple shear of dense frictional suspensions. *Journal of Rheology*, 62(2):457–468, 2018.
- [47] Jeffrey F Morris. Shear thickening of concentrated suspensions: Recent developments and relation to other phenomena. *Annual Review of Fluid Mechanics*, 52:121–144, 2020.
- [48] Ryohei Seto and Giulio G Giusteri. Normal stress differences in dense suspensions. *Journal of Fluid Mechanics*, 857:200–215, 2018.
- [49] Brice Lecampion and Dmitry I Garagash. Confined flow of suspensions modelled by a frictional rheology. *Journal of Fluid Mechanics*, 759:197–235, 2014.
- [50] Jurriaan JJ Gillissen and Christopher Ness. Modeling the microstructure and stress in dense suspensions under inhomogeneous flow. *Physical Review Letters*, 125(18):184503, 2020.
- [51] Wouter Peerbooms, Antoine van der Heijden, and Wim-Paul Breugem. Transient behavior and steady-state rheology of dense frictional suspensions in pressure-driven channel flow. *Acta Mechanica*, 236(9):5681–5714, 2025.
- [52] David Leighton and Andreas Acrivos. The shear-induced migration of particles in concentrated suspensions. *Journal of Fluid Mechanics*, 181:415–439, 1987.
- [53] Christopher J Koh, Philip Hookham, and L Gary Leal. An experimental investigation of concentrated suspension flows in a rectangular channel. *Journal of Fluid Mechanics*, 266:1–32, 1994.
- [54] Prabhu R Nott and John F Brady. Pressure-driven flow of suspensions: simulation and theory. *Journal of Fluid Mechanics*, 275:157–199, 1994.

- [55] Prabhu R Nott, Elisabeth Guazzelli, and Olivier Pouliquen. The suspension balance model revisited. *Physics of Fluids*, 23(4):043304, 2011.
- [56] Michel Orsi, Laurent Lobry, Elisabeth Lemaire, and François Peters. Mass and momentum balance during particle migration in the pressure-driven flow of frictional non-brownian suspensions. *Journal of Fluid Mechanics*, 998:A16, 2024.
- [57] Willian Hogendoorn, Wim-Paul Breugem, David Frank, Martin Bruschewski, Sven Grundmann, and Christian Poelma. From nearly homogeneous to core-peaking suspensions: Insight in suspension pipe flows using mri and dns. *Physical Review Fluids*, 8(12):124302, 2023.
- [58] Francesco Picano, Wim-Paul Breugem, Dhruvaditya Mitra, and Luca Brandt. Shear thickening in non-brownian suspensions: an excluded volume effect. *Physical review letters*, 111(9):098302, 2013.
- [59] Iman Lashgari, Francesco Picano, Wim Paul Breugem, and Luca Brandt. Channel flow of rigid sphere suspensions: particle dynamics in the inertial regime. *International Journal of Multiphase Flow*, 78:12–24, 2016.
- [60] JF Richarson and WN Zaki. Sedimentation and fluidisation: Part 1. *Trans. Ins. Chem. Eng*, 31:35–53, 1954.
- [61] John Garside and Maan R Al-Dibouni. Velocity-voidage relationships for fluidization and sedimentation in solid-liquid systems. *Industrial & engineering chemistry process design and development*, 16(2):206–214, 1977.
- [62] Xiaolong Yin and Donald L Koch. Hindered settling velocity and microstructure in suspensions of solid spheres with moderate reynolds numbers. *Physics of Fluids*, 19(9):093302, 2007.
- [63] Renzo Di Felice and Enrico Parodi. Wall effects on the sedimentation velocity of suspensions in viscous flow. *AIChE journal*, 42(4):927–931, 1996.
- [64] Alfred W Francis. Wall effect in falling ball method for viscosity. *Physics*, 4(11):403–406, 1933.
- [65] William L Haberman and Rose M Sayre. Motion of rigid and fluid spheres in stationary and moving liquids inside cylindrical tubes. Technical report, David Taylor Model Basin Washington DC, 1958.
- [66] M Coutanceau. Sur l'étude expérimentale de l'écoulement engendré par une sphere qui se déplace dans l'axe d'un cylindre au-dela du régime de stokes. *CR Acad. Sci. A*, 274:853–856, 1972.
- [67] Madeleine Coutanceau and Patrick Thizon. Wall effect on the bubble behaviour in highly viscous liquids. *Journal of Fluid Mechanics*, 107:339–373, 1981.
- [68] RP Chhabra, S Agarwal, and K Chaudhary. A note on wall effect on the terminal falling velocity of a sphere in quiescent newtonian media in cylindrical tubes. *Powder technology*, 129(1-3):53–58, 2003.

- [69] R Di Felice. A relationship for the wall effect on the settling velocity of a sphere at any flow regime. *International Journal of Multiphase Flow*, 22(3):527–533, 1996.
- [70] Elisabeth Guazzelli and John Hinch. Fluctuations and instability in sedimentation. *Annual review of fluid mechanics*, 43:97–116, 2011.
- [71] Russel E Caflisch and Jonathan HC Luke. Variance in the sedimentation speed of a suspension. *Physics of Fluids*, 28(3):759–760, 1985.
- [72] EJ Hinch. Sedimentation of small particles. In *Disorder and Mixing: Convection, Diffusion and Reaction in Random Materials and Processes*, pages 153–162. Springer, 1988.
- [73] Donald L Koch and ESG Shaqfeh. Screening in sedimenting suspensions. *Journal of fluid mechanics*, 224:275–303, 1991.
- [74] Anthony JC Ladd. Hydrodynamic screening in sedimenting suspensions of non-brownian spheres. *Physical review letters*, 76(8):1392, 1996.
- [75] Anthony JC Ladd. Sedimentation of homogeneous suspensions of non-brownian spheres. *Physics of Fluids*, 9(3):491–499, 1997.
- [76] Pedro Costa, Bendiks Jan Boersma, Jerry Westerweel, and Wim-Paul Breugem. Collision model for fully resolved simulations of flows laden with finite-size particles. *Physical Review E*, 92(5):053012, 2015.
- [77] Wim-Paul Breugem. A second-order accurate immersed boundary method for fully resolved simulations of particle-laden flows. *Journal of Computational Physics*, 231(13):4469–4498, 2012.
- [78] JC Brändle de Motta, Pedro Costa, Jacobus J Derksen, C Peng, L-P Wang, W-P Breugem, Jean-Luc Estivalèzes, Stéphane Vincent, E Climent, Pascal Fede, et al. Assessment of numerical methods for fully resolved simulations of particle-laden turbulent flows. *Computers & Fluids*, 179:1–14, 2019.

Viscous sedimentation of dense suspensions in narrow vertical tubes

Sedimentation of dense suspensions has been widely studied in systems that are large compared to the size of the particles. Much less is known about sedimentation in small systems, where the presence of walls has a pronounced effect on the dynamics. The objective of the present study is to gain understanding of the influence of confinement on sedimentation of dense suspensions of non-colloidal particles in narrow vertical tubes in the viscous flow regime. To this purpose, we have employed particle-resolved Direct Numerical Simulations (DNS) based on a computationally efficient Immersed Boundary Method (IBM) for the fluid/solid coupling and a frictional soft-sphere collision model for particle contact. We studied both the settling of a single particle and dense particle suspensions in the bulk concentration range of $0.05 \leq \phi_b \leq 0.3$. The influence of confinement was investigated for the range of $D/d = 2 - 11$, with D the tube diameter and d the diameter of the spherical particles. The mean sedimentation velocity, V_s , can be accurately described through a modified Richardson-Zaki correlation, with a prefactor $k \approx 0.8$ and with the terminal settling velocity for a single-settling particle in free space replaced by the Francis correlation for settling in a narrow tube. The particle rms velocities appear to scale with $V_s \phi_b^{1/3} (D/d)^{2/3}$ for $D/(d\phi_b^{-1/3}) \gtrsim 2.5$, while for smaller tubes the scaling behavior is very different due to strong confinement effects on the particle microstructure. For $D/(d\phi_b^{-1/3}) \gtrsim 2.5$, the Lagrangian lengthscale of correlated particle motions in the axial direction is proportional to $D\phi_b^{-1}$, and much larger than the Lagrangian length-scales in the other two directions, suggesting the presence of elongated vertical structures. All simulations showed a pronounced concentration peak at the wall, originating from particle-wall layering. The layering appears to extend into the tube with a second and smaller peak at a distance of $\approx 1.4d$. Interestingly, the particles around the internal concentration peak appear to settle significantly faster than the particles near the wall and in the core, especially for $\phi_b = 0.2$ and $D/d \geq 6$ for which the pdf of the vertical particle velocity also exhibits super-Gaussian behavior. This is indicative for streaming-like behavior of rather stable and vertically elongated particle clusters.

2.1 Introduction

Sedimentation (i.e., the collective settling of solid particles suspended in a fluid) is relevant to many different natural and industrial processes. The present study is motivated by extrusion 3D printing of dense suspensions in additive manufacturing of, e.g., ceramics, metals and energetic materials [2, 3, 4]. Unwanted sedimentation may take place in the print head and supply tube when the printer is idle, resulting in inhomogeneities in the final product when printing is resumed.

Sedimentation phenomena have been studied since many years already, both in the viscous [5, 6] and the inertial flow regime [7]. From a fundamental point of view, the complexity of sedimentation arises from long and short-range hydrodynamic multi-particle interactions and particle collisions. In the present study, we consider the influence of confinement (i.e., the influence of the tube wall) on particle sedimentation, which complicates matter and, as will be discussed below, is not well understood yet.

We consider the gravitational settling of a suspension of spheres in a vertical narrow cylindrical tube with a diameter D . The spheres are monodisperse with diameter d and have a mass density ρ_p . They are suspended in a Newtonian liquid with dynamic viscosity η_f and mass density ρ_f . Furthermore, the spheres are non-colloidal and non-Brownian (i.e., molecular forces between particles are negligible and $d \gg 1 \mu\text{m}$ such that the Péclet number based on the Brownian particle diffusivity is much larger than 1 [8]). Under these conditions, the sedimentation dynamics is governed by 4 dimensionless numbers: (1) the Galileo number, $Ga = \sqrt{|\bar{\rho} - 1| g d^3 / \nu_f^2}$, where g denotes the gravitational acceleration magnitude and $\nu_f = \eta_f / \rho_f$ is the kinematic fluid viscosity, (2) the particle/fluid density ratio, $\bar{\rho} = \rho_p / \rho_f$, (3) the particle-to-tube diameter ratio, $\lambda = d/D$, and (4) the bulk solid volume fraction, ϕ_b . We remark that sedimentation is often considered as dynamically similar to fluidisation [9, 10], assuming that the particle-mean settling velocity in sedimentation is equivalent to the superficial fluid velocity in fluidisation at the same ϕ_b . While this is true for $\lambda \ll 1$ (i.e., negligible wall effects), the similarity breaks down in narrow tubes: even when the relative particle/fluid velocity would be matched, the relative fluid/wall and particle/wall velocities will still be different between the two processes.

Single settling particle The presence of a wall has a retarding effect on sedimentation. This has been well documented for the case of a single settling sphere. For a sphere falling along the axis of a tube in the Stokes regime, exact analytical solutions have been derived for the ratio of the bounded, V_T , to the unbounded terminal settling velocity, $V_0 = V_T(\lambda \rightarrow 0)$. These solutions are either valid for sufficiently small λ [11] or for $\lambda \rightarrow 1$ [12]. Francis [13] proposed an empirical correlation that has a rather simple form:

$$\frac{V_T}{V_0} = \left(\frac{1 - \lambda}{1 - 0.475\lambda} \right)^4. \quad (2.1)$$

Interestingly, in his experiments on a steel ball settling in glycerol, he observed that the ball always settled along the wall instead of along the centerline of the tube, and that the ball was rotating along a horizontal axis such that the local ball velocity was highest at the side closest to the tube wall. Eccentric settling and rotation of the sphere was also occasionally observed in experiments by others, which for high λ was partially attributed to geometrical imperfections of the tube [14]. Nevertheless, Francis' correlation compares well with later

experiments of Fidleris and Whitmore [15] up to at least $\lambda = 0.4$. Moreover, his correlation appears also in good agreement [16] with a more complex algebraic analytical expression derived by Haberman and Sayre [17] for a concentrically falling sphere, accurate up to $\lambda \approx 0.5$ [18, 19]:

$$\frac{V_T}{V_0} = \frac{1 - 2.1050\lambda + 2.0865\lambda^3 - 1.7068\lambda^5 + 0.72603\lambda^6}{1 - 0.75857\lambda^5}. \quad (2.2)$$

The presence of a tube wall delays the transition from the viscous-dominated to the inertia-dominated regime. Based on a significant loss of fore-and-aft symmetry of the flow around a settling sphere in a tube, Coutanceau [18, 20] proposed an empirical correlation for the critical particle Reynolds, $Re_{Tc} = V_{Tc}d/\nu_f$, for the breakdown of the Stokes flow regime:

$$Re_{Tc} = \frac{20}{7}(1 - \lambda)^{-0.56} - 2.75 \quad (\lambda < 0.8). \quad (2.3)$$

Chhabra et al. [21] used a different criterion for Re_{Tc} , based on a significant deviation of the measured V_T from Equation (2.2). Their tabulated results for Re_{Tc} vary from $Re_{Tc} = 0.018$ for $\lambda = 0$ to $Re_{Tc} = 0.031$ for $\lambda = 0.5$ (using Equation (2.2) to relate Re_{Tc} to their critical values for $Re_0 = V_0d/\nu_f$, the terminal Reynolds number of a single particle settling in free space). These values are considerably smaller than the values predicted from Coutanceau's correlation, $Re_{Tc} = 0.11$ and 1.46 , respectively.

Beyond the Stokes regime, the retarding effect of the wall decreases for increasing Reynolds number, related to a more axially elongated wake structure. Several correlations for V_T/V_0 exist for the inertial regime, which agree reasonably well with experimental data for specific ranges in Re_T and λ [15, 21]. Worth noting, in this respect, is the correlation proposed by Di Felice [22] for the entire Reynolds number range and $\lambda \lesssim 0.9$, which proved to be reasonably accurate compared to other correlations for the inertial regime [21]:

$$\frac{V_T}{V_0} = \left(\frac{1 - \lambda}{1 - 0.33\lambda} \right)^\alpha \quad \text{with} \quad \alpha = \frac{33 + 0.85Re_0}{10 + Re_0}. \quad (2.4)$$

We remark that Re_0 can be related to Ga through $Re_0 = (2/\sqrt{3C_d})Ga$ with $C_d = C_d(Re_0)$ the drag coefficient of a sphere in free space. For $\lambda \rightarrow 0$ and $Re_0 \rightarrow 0$, Equation (2.4) reduces to $V_T/V_0 \approx 1 - 2.2\lambda$, which is fairly close to $V_T/V_0 \approx 1 - 2.1\lambda$ predicted from Equations (2.1) and (2.2) for the Stokes regime.

Collective settling of spheres Except for $\phi_b \lesssim 0.01$ at $Ga \gtrsim 155$ [23, 24, 25], the collective settling of spheres in a suspension is characterized by hindered settling, i.e., a reduction in the particle-averaged settling speed, V_s , with increasing particle concentration [10, 26, 5, 27]. A widely used correlation for hindered settling is the one proposed by Richardson and Zaki [9]:

$$V_s = kV_0(1 - \phi_b)^n, \quad (2.5)$$

with $k = k(\lambda)$, and $n = n(Re_0, \lambda)$. The coefficient k was found to be different for sedimentation as compared to fluidisation. According to Richardson and Zaki [9]:

$$k = 1 \quad \text{for sedimentation,} \quad (2.6a)$$

$$k = 10^{-\lambda} \quad \text{for fluidisation.} \quad (2.6b)$$

Furthermore, for $Re_0 < 1$, the following correlations were proposed for the exponent n :

$$Re_0 < 0.2 \quad : \quad n = 4.65 + 19.5\lambda, \quad (2.7a)$$

$$0.2 < Re_0 < 1 \quad : \quad n = (4.35 + 17.5\lambda)Re_0^{0.03}. \quad (2.7b)$$

Note that these correlations for n are discontinuous at $Re_0 = 0.2$. Furthermore, λ was smaller than 0.04 in the experiments of Richardson and Zaki for the range of $Re_0 < 1$. Also, no measurements were performed in the dilute regime; the values for kV_0 and n were obtained from fitting Equation (2.5) for $\phi_b \gtrsim 0.05$, and dividing kV_0 by a theoretical estimate of V_0 to estimate k .

Garside and Al-Dibouni [26] critically evaluated the Richardson-Zaki correlation and proposed new correlations for k and n that more accurately capture the abundance of experimental data:

$$k = (1 + 2.35\lambda)^{-1}, \quad (2.8a)$$

$$n = \frac{5.1 + 0.27Re_T^{0.9}}{1 + 0.1Re_T^{0.9}} \quad (2.8b)$$

where Re_T was determined from $Re_T = kRe_0$, using k from Equation (2.8a) and estimating Re_0 from drag correlations for a single settling sphere in free space. Differences of their modified correlation with the original Richardson-Zaki correlation are that $k < 1$ and decreases with increasing λ without making distinction between fluidisation and sedimentation, and that n depends only on Re_T instead of on Re_0 and λ . As explained before, the presence of a wall breaks the similarity between fluidisation and sedimentation, and it is therefore counter-intuitive that the same correlation holds for both flow types.

Di Felice and Parodi [28] noticed that Equation (2.7a) is actually the result of a poor correlation. By neglecting two outliers in the underlying dataset, they concluded that n is hardly affected by λ and in the range of $n \approx 4.7 - 4.9$. In addition, they performed experiments in the Stokes regime for both low concentrations ($\phi_b = 0 - 0.05$, the range not measured by Richardson and Zaki) and high concentrations ($\phi_b = 0.1 - 0.35$). For the *low* concentrations, both n and k sharply decreased with λ , with n varying from $n \approx 6.5$ at $\lambda = 0.05$ to $n \approx 2.3$ at $\lambda = 0.2$, and $k \approx V_T/V_0$ with V_T/V_0 given by Equation (2.1). In contrast, for the *high* concentrations, both n and k were nearly independent of λ , with $n \approx 4.6 - 4.8$ and $k \approx 0.8$. Although the value found for n is in agreement with the redetermined value for n from the data of Richardson and Zaki, the value of k is significantly lower than $k \approx 1$ as suggested by Richardson and Zaki for sedimentation. Furthermore, the findings of Di Felice and Parodi contradict the correlation for k proposed by Garside and Al-Dibouni, Equation (2.8a), which predicts the same dependence on λ for the entire concentration range.

Particle velocity fluctuations Sedimenting suspensions are characterized by relatively strong particle velocity fluctuations akin of turbulent convection [29]. The influence of confinement on particle velocity fluctuations and related particle self-diffusion, has received considerable attention in literature, especially for dilute suspensions in the Stokes regime [6]. This was triggered by theoretical predictions [30, 31, 32] and Lattice-Boltzmann simulations of sedimentation in a triply periodic domain [33, 34] that for a

random particle distribution, the velocity variance diverges linearly with the size of the system in which the sedimentation process takes place. The divergence originates from long-range hydrodynamic interactions between particles, which scale with $\sim V_{st}d/r$ in the Stokes regime, where $V_{st} = (1/18)(\rho_p - \rho_f)gd^2/\eta_f$ is the Stokes velocity for a single sphere settling in free space and r denotes the radial distance from a particle to a neighboring particle. In contrast, sedimentation experiments by Nicolai and Guazzelli [35] showed that the fluctuations are independent of system size for L/d in the range of $\approx 25 - 100$ (with L the shortest horizontal dimension of the rectangular containers used). The apparent controversy between theory, simulations and experiments has become known as the ‘divergence paradox’.

The conceptual theory of Hinch [31, 6] provided already a clue to resolve the controversy. He postulated that sedimentation is characterized by ‘blobs’ of correlated particle motions. For a random particle distribution, the number of particles in a spherical blob with size l is expected to exhibit a Poisson distribution with a mean of $N = \phi_b(l/d)^3$ and a standard deviation proportional to $\sqrt{N}$ [36, 37, 38]. The fluctuations in the number of particles within the blobs are responsible for density fluctuations, causing heavier blobs to sink and lighter blobs to rise with respect to the mean sedimentation speed. By balancing the blob weight with Stokes drag acting on the blob, he found that the velocity fluctuation of a blob scales as $\sim V_{st}\sqrt{\phi_b}l/d$. This finding suggests that the particle velocity variance scales linearly with the shortest system size L as this limits the maximum possible blob size, in agreement with the theoretical prediction of Caflisch and Luke [30]. Interestingly, Hinch suggested that the scaling with system size only holds for the initial stage of sedimentation. He speculated that ‘after some time’ convective motions would ‘remove’ large-scale density variations down to an ‘irreducible’ scale on the order of the interparticle distance $\sim (d/2)\phi_b^{-1/3}$, thus independent of system size. His speculation was later supported by experimental results of Guazzelli [39] for sedimentation of dilute suspensions in a large container ($L/d \approx 500$ and ≈ 675 for the two different particle batches used). While the initial fluctuating particle motions exhibited a lengthscale on the order of the system size, the lengthscale was found to decrease over time down to a characteristic blob size of 15 to 20 times $(d/2)\phi_b^{-1/3}$ at flow equilibrium.

Lattice Boltzmann simulations by Ladd [40] and Nguyen and Ladd [41] of sedimentation in a rectangular container at $\phi_b = 0.13$ and, respectively, a Reynolds number $V_s d/\nu_f = 0.2$ and 0.06 , highlighted the importance of impenetrable bottom and top walls on the particle velocity fluctuations. While the particle rms velocity was found to diverge with increasing container width when periodic boundary conditions were used in the vertical direction, the rms velocity reached a constant value for sufficiently large container width when no-slip walls were used in the vertical direction [40]. The presence of the bounding walls was shown to gradually reduce the particle rms velocity until equilibrium was reached [40] and to strongly damp large-scale horizontal density fluctuations over the course of the sedimentation process [41]. They suggested that the initial large-scale density fluctuations are convected towards either the bottom or the top of the sedimenting suspension and adsorbed by the density gradient at the interface with, respectively, the bed and the supernatant, in line with the speculation made earlier by Hinch [31].

For dilute suspensions in the Stokes regime, Segrè et al. [42] found a profound influ-

ence of container size on the rms of the particle velocity fluctuations according to:

$$\frac{V_{rms}}{V_s} = C_1 \phi_b^{1/3} [1 - \exp(-L/(C_2(d/2)\phi_b^{-1/3}))], \quad (2.9)$$

2

where C_1 and C_2 are constants with $C_1 \approx 1$ for horizontal and ≈ 2 for vertical velocity fluctuations and $C_2 \approx 60$, and L denotes either the container width or radius dependent on the container shape (rectangular or cylindrical) in their sedimentation experiments. For a given bulk concentration, confinement is thus responsible for a reduction in the relative rms velocity with respect to the asymptotic value for very large containers. Equation (2.9) fitted well with previous experimental results of Nicolai et al. [35] and Ham and Homsy [43] for relatively small containers. Finally, for $L > 150(d/2)\phi_b^{-1/3}$ it was found from a spatial correlation analysis that the blobs have a column-like shape with a height of $\approx 22(d/2)\phi_b^{-1/3}$ and a diameter of $\approx 27(d/2)\phi_b^{-1/3}$, implying that in large systems the blobs contain ≈ 3000 particles on average, irrespective of the bulk concentration.

Surprisingly, Segrè et al. [42] obtained their correlation by equating the system size L in Equation (2.9) to the largest horizontal dimension (width) of the rectangular containers used in their experiments. As pointed out by Brenner [44], the blob dimensions determined for the largest containers always exceeded half the value of the shortest horizontal dimension (half-depth) of the containers, suggesting a non-negligible effect from the walls. Assuming that the blobs are traversing across the depth of the container, Brenner proposed an alternative theory that reproduces the power-law scaling of the blob size and the relative rms velocity in the bulk concentration as found by Segrè et al. [42] for their largest systems, but which does include a dependency on the system depth.

Segrè et al. [45] extended the conceptual theory of Hinch [31] to the dense regime by (a) replacing the Stokes velocity by the actual sedimentation velocity, (b) replacing the fluid viscosity by the suspension viscosity, and (c) by accounting for an excluded volume effect in the estimate of the fluctuating mass of a blob. Their model showed good agreement with measured rms velocities of sedimenting particles in a large container (large in terms of the criterion proposed by Segrè et al. [42]), and captured the fairly constant relative rms velocity over a large range in concentration and the decrease at very high concentrations beyond $\phi_b \approx 0.3$. Furthermore, a spatial correlation analysis of the particle velocity fluctuations indicated that the characteristic blob dimensions in the dense regime are identical to blob dimension in the dilute regime, a remarkable and unexpected result [46]. In contrast, Snabre et al. [47] measured a strong increase in the spatial correlation length for concentrations beyond $\phi_b \approx 0.5$, indicative of a jamming transition. They attributed this to the smaller particle/fluid density difference in their experiments as compared to Segrè et al. [45].

Inertial effects A number of studies addressed the influence of inertia when the particle Reynolds number is gradually increased beyond the Stokes regime, using theory [31, 48, 44], numerical simulations [49, 50, 51, 52, 53, 7] and experiments [37]. Lattice-Boltzmann simulations by Yin and Koch [51] highlighted the importance of wake-induced particle-particle interactions and related drafting-kissing-tumbling behavior [54] at finite particle Reynolds number in dilute suspensions, which were held responsible for the observed deviation of the microstructure from an isotropic ‘hard-sphere’ distribution [55, 8]. For dilute suspensions, Sungkorn and Derksen [53] and Yin and Koch [52] reported a

decrease in the relative rms velocity with increasing particle Reynolds number beyond $Re_T \approx 0.1$. Furthermore, Sungkorn and Derksen [53] found that the relative particle rms velocity can be described well with Equation (2.9) combined with empirical power-law expressions of the coefficients C_1 and C_2 as function of Re_T and ϕ_b . Worth mentioning is also their finding that the relative particle rms velocity reached a constant value for sufficiently long simulation time and for sufficiently large size of the triply periodic cubic domain used.

Bergounoux and Guazzelli [37] performed experiments on dilute sedimenting suspensions with very low Re_T pertaining to the Stokes regime, but with $Re_L = Re_T(L/d)$ in the range of 0.01 – 24.1. The suspension microstructure was found to clearly depart from a random (Poisson) distribution for increasing Re_L , while the characteristic blob size remained constant at 15 to 20 times $(d/2)\phi_b^{-1/3}$. Interestingly, beyond $Re_L \approx 0.1$ the relative particle rms velocity started to decrease from the plateau value for the Stokes regime according to $\sim Re_L^{-0.1}$. The conceptual theory of Hinch [31] was adjusted by accounting for weak inertial effects and captured the observed drop in the rms velocity fairly well.

In a recent study on inertial effects in sedimentation, Shajahan and Breugem [7] distinguished between a dilute ($\phi_b \lesssim 0.02$), moderately dense ($0.02 \lesssim \phi_b \lesssim 0.1$) and dense suspension regime ($\phi_b \gtrsim 0.1$), each characterized by a different microstructure and sedimentation dynamics. Remarkably, their particle-resolved Direct Numerical Simulations (DNS) for the range of $Ga = 144 - 210$ showed little influence of inertia when $\phi_b \gtrsim 0.02$, which was attributed to the ‘obstruction and perturbation of the particle wake by neighboring particles’. Drafting-kissing-tumbling was found to dominate the suspension behavior in the moderately dense regime and responsible for a preferential settling of particles in horizontal pairs at a distance of $\sim 1.5d$. In contrast, a nearly isotropic hard-sphere distribution was observed in the dense regime, dominated by short-range (lubricated) multi-particle interactions.

Intrinsic convection Finally, sedimenting suspensions in closed containers are prone to a phenomenon known as intrinsic convection, at least in the dilute regime [56]. Intrinsic convection originates from the presence of buoyant particle-depleted wall layers [57, 58, 59], causing a reduced sedimentation velocity of the particles near the container walls. Mass conservation requires an enhanced sedimentation speed in the core. Peysson and Guazzelli [60] found evidence for intrinsic convection at $\phi_b = 0.1$ and 0.2 in the Stokes regime, but much weaker than predicted by theory for dilute suspensions [61, 62]. It was suggested that this is an effect of the observed concentrated particle-wall layers and related particle-particle and particle-wall interactions in the experiments, which is not fully accounted for in the theory. If intrinsic convection is present, then an inhomogeneous particle velocity distribution may be expected, dependent on the distance to the nearby wall(s).

From the above literature review, it is clear that the effect of confinement on particle sedimentation is far from understood. Conflicting correlations have been proposed for n and k . Furthermore, the presence of convection structures and the heterogeneous spatial particle distribution complicate the sedimentation dynamics in confined geometries. Finally, little research has been performed yet on sedimentation under strong confinement (i.e., for the range of relatively high λ).

The objective of the present study is to gain understanding of the influence of con-

finement on sedimentation of dense particle suspensions in narrow vertical tubes in the viscous flow regime. To this purpose, we have employed particle-resolved Direct Numerical Simulations (DNS) based on a computationally efficient Immersed Boundary Method (IBM) for the fluid/solid coupling [63] and a frictional soft-sphere collision model [64] for particle collisions. We studied both the settling of a single particle and the sedimentation of dense particle suspensions in the concentration range of $0.05 \leq \phi_b \leq 0.3$. The influence of confinement was investigated for the range of $D/d = 2 - 11$ corresponding to $0.091 \leq \lambda \leq 0.5$. Furthermore, for the chosen parameter ranges, $D/(0.5d\phi_b^{-1/3})$ varies from 1.5 (for $\phi_b = 0.05$ and $D/d = 2$) to 12.9 (for $\phi_b = 0.2$ and $D/d = 11$). The tube diameter is thus always smaller than the characteristic blob size of 15 to 20 times $(d/2)\phi_b^{-1/3}$ reported in literature for unconfined sedimentation [37, 65]. Hence, a strong effect of the tube wall may be expected on the sedimentation dynamics as well as a radially dependent particle concentration and velocity distribution. The sedimentation dynamics is analyzed in terms of particle statistics, including the mean and rms particle velocities, the radial particle distribution, particle dispersion characteristics and particle clustering in the vertical direction. With these statistics we obtain both a clear picture of the macroscopic suspension behavior as well as insight in the underlying suspension microstructure.

The remainder of this chapter is organized as follows. In Section 2.2, the governing equations are introduced and details of the contact model are given. In Section 2.3, the numerical method and computational setup are described. In Sections 2.4.1 and 2.4.2, the DNS results are presented for, respectively, the settling of a single sphere and the sedimentation of a dense suspension in a narrow tube. Finally, in Section 2.5, the main findings are summarized, followed by a discussion and recommendations for future research.

2.2 Governing equations and contact model

The fluid phase is governed by the incompressible Navier-Stokes equations that are made dimensionless with the following reference scales: $l_{\text{ref}} = d$, $u_{\text{ref}} = \sqrt{gd}$, and $t_{\text{ref}} = l_{\text{ref}}/u_{\text{ref}}$. This leads to the following equations:

$$\nabla \cdot \mathbf{u} = 0, \quad (2.10a)$$

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot \mathbf{u}\mathbf{u} = -\nabla p_h - \nabla p + \frac{\sqrt{|\bar{\rho} - 1|}}{Ga} \nabla^2 \mathbf{u}, \quad (2.10b)$$

in which $\mathbf{u}$ is the velocity, p_h represents the linearly varying part of the absolute pressure (p_{abs}) over the tube height related to the presence of particles, and p is the modified pressure defined by $p = p_{\text{abs}} - p_h - \tilde{\mathbf{g}} \cdot \mathbf{x}$ with $\tilde{\mathbf{g}} = \mathbf{g}/|\mathbf{g}|$ the unit vector pointing in the direction of gravity. The gradient in p_h is dynamically adjusted to enforce that the overall mixture bulk velocity is zero; this mimics sedimentation in a closed tube. Based on an overall vertical force balance, ∇p_h balances the submerged weight of the particles in suspension, the fluid wall shear stress and possible solid friction from particle/wall contacts.

The translational ($\mathbf{u}_p$) and the angular particle velocity ($\boldsymbol{\omega}_p$) of the spherical particles are determined from solving the Newton-Euler equations, respectively:

$$\frac{\pi}{6} \bar{\rho} \frac{d\mathbf{u}_p}{dt} = \oint_{\partial V} (\boldsymbol{\sigma}_f \cdot \mathbf{n}) dA + \frac{\pi}{6} ((\pi_p - 1) \sim \tilde{\mathbf{g}} - \nabla p_h) + \mathbf{F}_c, \quad (2.11a)$$

$$\frac{\pi}{60}\bar{\rho}\frac{d\omega_p}{dt} = \oint_{\partial V} \mathbf{r} \times (\boldsymbol{\sigma}_f \cdot \mathbf{n}) dA + \mathbf{T}_c. \quad (2.11b)$$

The fluid stress tensor is defined as $\boldsymbol{\sigma}_f = -p\mathbf{I} + (\sqrt{|\bar{\rho}-1|/Ga})((\nabla\mathbf{u}) + (\nabla\mathbf{u})^T)$, where $\mathbf{n}$ is the outward pointing normal vector on the particle surface ∂V , and $\mathbf{r}$ is the position vector with respect to the particle centroid. $\mathbf{F}_c$ and $\mathbf{T}_c$, are, respectively, the force and torque working on the particle as a result of collisions with other particles or the tube wall.

The fluid and particle equations are coupled with each other through the no-slip/no-penetration condition at the surface of the particles:

$$\mathbf{u} = \mathbf{u}_p + \boldsymbol{\omega}_p \times \mathbf{r} \quad \text{on } \partial V. \quad (2.12)$$

Particle collisions and contacts are modelled through a frictional soft-sphere collision model [64]. This is a linear spring-dashpot model in which the *rigid* particles are *numerically* allowed to overlap slightly. For each colliding particle pair, the collision force is computed from the overlap between the two particles and their relative velocity. The model accounts for stick/slip transition dependent on the ratio of the tangential to the normal collision force component. The expressions for the normal and tangential force components are given by, respectively:

$$\mathbf{F}_n = -k_n\boldsymbol{\delta}_n - \eta_n\mathbf{u}_n, \quad (2.13a)$$

$$\mathbf{F}_t = \min(\| -k_t\boldsymbol{\delta}_t - \eta_t\mathbf{u}_t \|, \| -\mu_c\mathbf{F}_n \|) \mathbf{t}. \quad (2.13b)$$

Here, $\boldsymbol{\delta}_n$ is the overlap between the two particles, $\mathbf{u}_n$ is the relative normal velocity, k_n is the normal spring stiffness coefficient, and η_n is the normal damping coefficient. Similarly, $\boldsymbol{\delta}_t$ is the tangential displacement between the particles in their point of contact, $\mathbf{u}_t$ is the relative tangential velocity, k_t is the tangential spring stiffness coefficient, η_t is the tangential damping coefficient, and $\mathbf{t}$ is the tangent unit vector that indicates the direction of the tangent collision force. Once the collision force is computed, the collision torque is calculated according to $\mathbf{T}_c = \mathbf{r} \times \mathbf{F}_t$, where $\mathbf{r}$ denotes here the radius vector pointing from the particle centroid towards the point of contact between the particles.

The collision parameters k_n , η_n , k_t , and η_t are determined from analytical expressions that depend on the reduced mass of the particles, the tangential and normal dry coefficients of restitution (e_t and e_n , respectively), and the collision time (ΔT_c). The latter is a numerical parameter; this allows for artificially stretching the collision time in order to avoid excessively small time steps for resolving collision events. Similar to the values used in the DNS studies of Hogendoorn et al. [66] and Shajahan et al. [67], we used $e_t = 0.1$, $e_n = 0.97$ and $\Delta T_c = 8\Delta t$, where Δt is the computational time step. Furthermore, the Coulomb friction coefficient is set to $\mu_c = 0.39$.

2.3 Numerical method and computational setup

In the DNS, the governing equations for the fluid phase are solved on a fixed Cartesian grid with a second-order accurate finite-volume/central-differencing scheme. A computationally efficient Immersed Boundary Method (IBM) [63] is employed for the fluid/solid coupling, in which the no-slip/no-penetration condition at the surface of the particles is enforced by good approximation by locally adding forces to the right-hand side of Equation

(2.10b). The IBM makes use of a Lagrangian grid attached to the surface of the particles and a regularized Dirac delta function to interpolate values from the Eulerian fluid grid to the Lagrangian particle grid and vice versa. As in previous particle-laden pipe flow studies [66, 67], a volume-penalization IBM [68] is adopted for imposing the no-slip/no-penetration condition on the tube wall. The Navier-Stokes and Newton-Euler equations are integrated in time with the third-order Runge-Kutta 3 (RK3) scheme using the same computational step for both the fluid and the particle phase. For more details and validation of our approach, the reader is referred to [63, 66, 67]. For the present study, we used a uniform grid resolution of $d/\Delta x = 16$, which corresponds to 746 Lagrangian grid cells on the surface of each particle. The time step is fixed at $\Delta t \sqrt{g/d} = 5.1 \cdot 10^{-3}$. Finally, we add a lubrication force correction to the right-hand side of Equation (2.11b) when two neighboring particles are separated less than one grid cell apart to compensate for the lack of local grid resolution [64, 69, 70]. The correction is based on an asymptotic solution for the normal force on two approaching particles in the Stokes regime. The diverging behavior of the force correction is capped when the distance between the particles drops below $10^{-3}d$, which, from a physical point of view, mimics the effect of typical particle surface roughness on the lubrication dynamics.

The initial particle positions were randomly distributed inside the tube by inserting particles into the pipe one after the other, while ensuring no overlap between the particles and between the particles and the tube wall. The particles and the fluid were initialized with zero velocity in the entire domain. Directly at the start of the simulations, the particles are allowed to settle under gravity in the vertical direction. To prevent the influence of the periodic boundary conditions imposed in the vertical direction, a sufficiently long vertical pipe was used in the DNS, varying in length from $L_y/d = 105$ to 420 between the different cases. The background pressure gradient in Equation (2.10b), ∇p_h , was dynamically adjusted to enforce a zero mixture (fluid + particles) bulk velocity in the vertical direction. This mimics the presence of a bottom wall in our setup.

In our simulations, the density ratio and Galileo number were fixed at $\bar{\rho} = 1.05$ and $Ga = \sqrt{18} \approx 4.2$, respectively. These values are representative for polystyrene particles with a diameter of 0.33 mm in water at room temperature. We note that the Galileo number $Ga = \sqrt{18}$ corresponds to a Reynolds number $V_{St}d/\nu_f = 1$ based on the Stokes velocity, which is the very same Reynolds number considered by Kuusela et al. [50] in their study of sedimentation of dense sphere suspensions between two parallel plates. Using Beard's correlation [16] for the sphere drag coefficient in the range of $0.01 < Re_0 < 20$, $C_d = (24/Re_0) \cdot \left(1 + 0.1315 Re_0^{[0.82-0.05w]}\right)$ with $w = \log_{10} Re_0$, our value of the Galileo number corresponds to an estimated Reynolds number of a single settling particle *in free space* of $Re_0 \approx 0.893$. Though this value of the Reynolds number pertains to the weakly inertial regime, the effective particle settling Reynolds number in our simulations is considerably lower due to effects of both confinement and hindered settling at finite concentration. The reasons for choosing here $Ga = O(1)$ instead of $Ga \ll 1$, are to avoid an excessively small computational time step and an excessively long simulation time for the system to reach equilibrium.

In the present study, we consider both the settling of a single particle for tube-to-particle diameter ratios in the range of $D/d = 2 - 20$ ($\lambda = 0.05 - 0.5$), and the settling of dense particle suspensions in the range of $D/d = 2 - 11$ ($\lambda = 0.091 - 0.5$) and $\phi_b = 0.05 - 0.3$.

In total 12 different simulations of sedimenting suspensions were conducted. Table 2.1 displays an overview of the different cases and simulation parameters. There are three things to note for these cases. First, for $D/d = 2$, the highest investigated concentration is $\phi_b = 0.1925$. This value is slightly below the value of 0.2 used for the higher D/d values. This was due to the small tube diameter in this case, for which we did not succeed to create a random initial distribution of particles at $\phi_b = 0.2$ with our injection approach. In the analysis of the results, we grouped this case with the other cases with $\phi_b = 0.2$ in order to study the effect of confinement on the sedimentation dynamics at constant bulk concentration. Second, $\phi_b = 0.3$ was simulated only in combination with $D/d = 4$ as this concentration could not be realized for lower D/d values with our injection method and since it was computationally expensive for higher D/d values. Third, dependent on the value of D/d , we varied the length of pipe in the vertical direction. For $D/d = 2$, a long pipe length was chosen to increase the number of particles in the domain and to improve statistical convergence of the computed particle statistics. For increasing D/d , a shorter pipe length was selected to limit the computational costs of the simulations.

For each simulation case, Table 2.1 also shows the Reynolds number based on the tube diameter and mean sedimentation velocity in the statistically steady state of the simulation, $Re_D = V_s D / \nu_f$. Additionally, the table contains a proxy for the vertical decorrelation lengthscale normalized by the particle diameter, $V_s \tau_{L,y} / d$, where V_s is the mean vertical velocity of the settling particles and $\tau_{L,y}$ is the integral timescale obtained from the time integral of the temporal autocorrelation of the vertical particle velocity fluctuations with respect to the mean vertical particle velocity. This proxy for the decorrelation length is used to check, a posteriori, that the chosen domain length was indeed sufficiently long to exclude any interaction of particles with themselves across the periodic boundaries in the vertical direction. Finally, the last four columns of Table 2.1 indicate the simulation timestep, development time, duration of the statistically steady state of the simulations, and the sampling interval for steady-state statistics.

Table 2.1: Parameters of the DNS cases of sedimenting dense suspensions in a narrow tube: D/d is the ratio between the tube diameter (D) and particle diameter (d), ϕ_b is the bulk solid volume fraction, L_y/d is the non-dimensional length of the domain in the direction of gravity, N_p is the number of particles, $Re_D = V_s D / \nu_f$ is the tube Reynolds number based on the tube diameter and mean sedimentation velocity, $V_s \tau_{L,y} / d$ is the integral lengthscale, $\Delta t_{sim} / t_{St}$ is the simulation timestep, t_{dev} / t_{St} is the flow development time, t_{stats} / t_{St} is the duration of the statistically steady state of the simulations, and $\Delta t_{stats} / t_{St}$ is the sampling interval for steady-state statistics.

D/d	ϕ_b	L_y/d	N_p	Re_D	$\frac{V_s \tau_{L,y}}{d}$	$\frac{\Delta t_{sim}}{t_{St}}$	$\frac{t_{dev}}{t_{St}}$	$\frac{t_{stats}}{t_{St}}$	$\frac{\Delta t_{stats}}{t_{St}}$
2	0.05	420	126	0.0121	16.6	0.00054	N/A	N/A	N/A
2	0.10	420	252	0.0054	3.5	0.00054	1074	343	0.269
2	0.1925	420	485	0.0048	1.6	0.00054	322	408	0.269
4	0.10	210	504	0.0436	5.9	0.00054	537	241	0.269
4	0.20	210	1008	0.0286	2.0	0.00054	376	311	0.269
4	0.30	210	1512	0.0158	1.1	0.00054	215	305	0.269
6	0.10	210	1134	0.0931	7.3	0.00054	430	214	0.269
6	0.20	210	2268	0.0570	2.6	0.00054	430	214	0.269
8	0.10	210	2016	0.1388	6.8	0.00054	430	214	0.269
8	0.20	210	4032	0.0859	2.8	0.00054	430	214	0.269
11	0.10	105	1906	0.2066	6.7	0.00054	430	214	0.269
11	0.20	105	3812	0.1264	3.4	0.00054	430	214	0.269

2.4 Results and discussion

2.4.1 Settling of a single sphere

In the single-particle simulations, a particle was placed at the center of a long tube and allowed to settle under gravity. The simulations were stopped when the particle reached its final equilibrium velocity. In all cases, the particle remained at the tube centerline. Figure 2.1 shows the terminal settling velocity of the particle as a function of the tube-to-particle diameter ratio D/d . The lines show various correlations from the literature, and the legend shows the corresponding values of V_0/V_{St} determined from a least-squares fit to the DNS data, where V_0 is the settling velocity for $D/d \rightarrow \infty$ and V_{St} is the Stokes velocity.

As expected, the particle settles faster (V_T becomes more negative) for increasing D/d . Over the entire D/d range investigated, our data shows good agreement with the correlations proposed by Francis [13], Haberman and Sayre [17] and Di Felice [22] as given by, respectively, Equations (2.1), (2.2), and (2.4). The correlations proposed by Richardson and Zaki [9], Equation (2.6b), and Garside and Al-Dibouni, Equation (2.8a), do not describe our data well over the entire range of D/d considered in this work.

Finally, the good agreement of our data with the empirical correlation of Francis [13] and the analytical expression of Haberman and Sayre [17], both established for the Stokes regime, indicates that the influence of confinement on the sphere settling velocity is stronger than possible inertial effects for the weakly inertial regime.

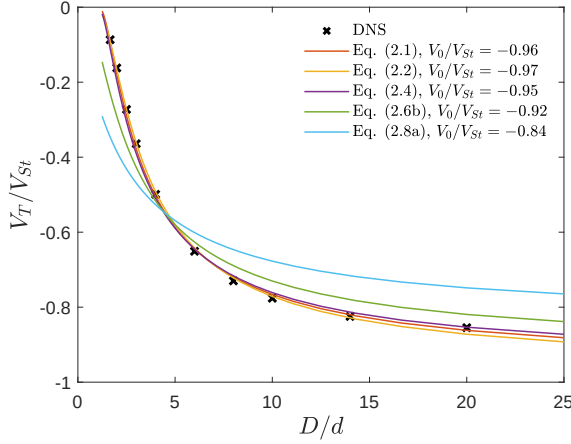


Figure 2.1: Terminal settling velocity of a single particle settling in a vertical tube, normalized by the Stokes velocity and shown as a function of tube-to-particle diameter ratio (D/d). The symbols represent the DNS results. The lines show various correlations from the literature with the corresponding values of V_0/V_{St} determined from a least-squares fit to the DNS data.

2.4.2 Sedimenting suspensions

Time-averaged quantities were calculated for the statistically steady state of the simulations. The start of the steady state was determined based on the development of the particle-averaged vertical velocity, the rms of the vertical particle velocity, and the mean radial position of the particles. These quantities are shown in Figure 2.2 for the cases with $D/d = 4$ as an example, with vertical lines indicating the start of the steady state. The time is normalized with the Stokes time defined as $t_{st} = (d/2)/V_{st}$. This figure shows that the transient is longer for lower solid volume fraction. Table 2.1 lists the development time for each case, as well as the duration of the steady state used for the calculation of statistics in the remainder of this work. For $D/d = 2$ and $\phi_b = 0.05$, the transient stage took long and the simulation was aborted before the steady state was reached.

To gain insight in the **spatial particle distribution during the flow development**, a visual representation of the suspensions is made. Figure 2.3 shows a series of snapshots of the sedimenting particles at a bulk volume fractions of $\phi_b = 0.1$ (a,b,c) and 0.2 (d,e,f), in a segment of the tube with a height of 50 particle diameters. Three diameter ratios are shown: (a,d) $D/d = 2$, (b,e) $D/d = 4$, and (c,f) $D/d = 8$, each at 5 different time instants (from left to right in each subfigure: $t = 0$, $t = 0.25t_{dev}$, $t = 0.5t_{dev}$, $t = 0.75t_{dev}$, and $t = t_{dev}$). The colors of the particles indicate the relative velocity fluctuations of the particles, defined as $V'_{rel} = (V - V_{mean})/V_{rms}$, where positive values of V'_{rel} correspond to particles sedimenting slower than the mean particle velocity and negative values correspond to particles sedimenting faster than the mean particle velocity. This coloring highlights clusters of particles that sediment with the same velocity to be able to see emerging structures in the suspension. It is interesting to note that, in the vertical direction, the sedimenting suspensions form clusters and depleted zones despite the random initial positioning. This effect is strongest for the small diameter ratio cases and becomes less distinct at larger

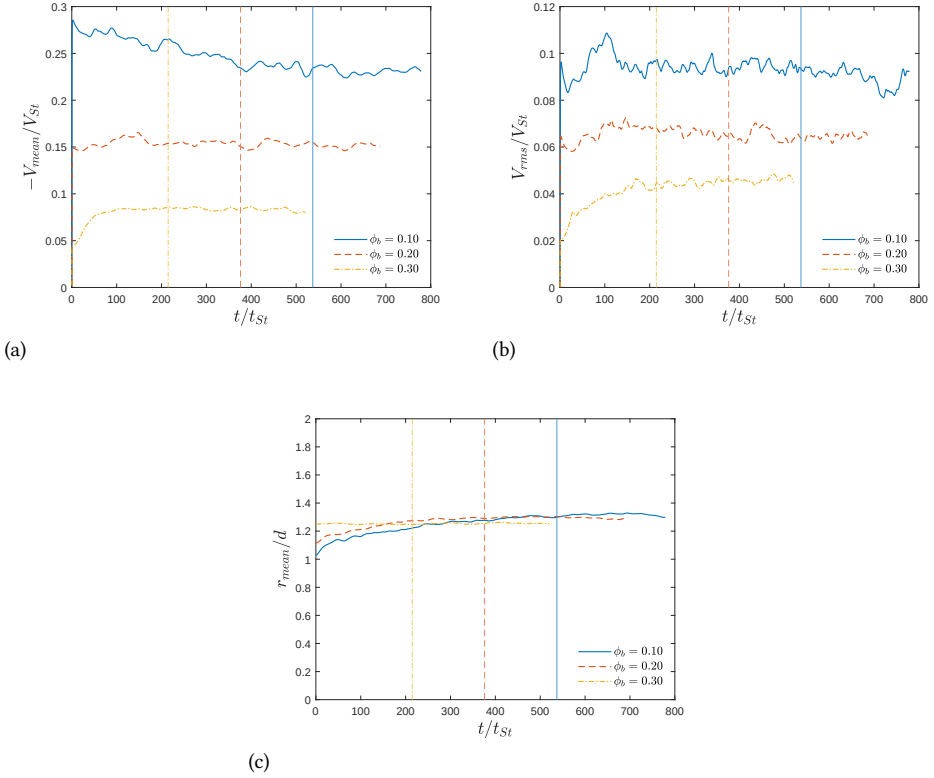


Figure 2.2: Temporal evolution of the particle-averaged vertical velocity (a), the rms of the vertical particle velocity (b), and the mean radial position of the particles (c) for the cases with $D/d = 4$. The vertical lines specify the start of the steady state.

diameter ratio. Next to the longitudinal clustering, the figure shows lateral movement of the particles. The particles collectively move closer to the wall over time, and locally it can be seen that there is a variation in particle concentration in the horizontal plane (XZ-plane). From Figure 2.3a ($D/d = 2$ and $\phi_b = 0.1$), it becomes clear that, in this very narrow tube, single particles and pairs of two particles fall slightly faster than the mean, whereas clusters of three or more particles fall slower than the mean. In Figure 2.3b ($D/d = 4$ and $\phi_b = 0.1$), some larger clusters with the same color can be observed, as well as preferential alignment in the vertical direction. For instance, in the third time instant ($t = 0.5t_{dev}$), a vertical train of bright yellow particles can be seen in the lower half of the tube. These particles settle with a velocity of up to $V_{mean} - 3V_{rms}$, which is more than double the mean velocity. In Figure 2.3c ($D/d = 8$ and $\phi_b = 0.1$), preferential alignment in the vertical direction is also clearly visible. Additionally, larger clusters with the same color can be observed, which seem to locally span across the entire pipe cross-section. For the cases with higher bulk particle concentration, Figure 2.3d ($D/d = 2$ and $\phi_b = 0.2$) shows similar behavior as observed for the lower concentration, with clusters falling slower than the

mean and single particles and doublets falling faster than the mean, with some particles exceeding velocities of $V_{mean} - 3V_{rms}$. The clusters that occur are larger in the vertical direction and consist of more particles as expected for a higher bulk volume concentration. Figure 2.3e ($D/d = 4$ and $\phi_b = 0.2$), also shows vertical alignment of particles with the same velocity, comparable to the lower concentration case. Additionally, some larger clusters can be observed that occupy more of the tube cross-section. The case shown in Figure 2.3f ($D/d = 8$ and $\phi_b = 0.2$) exhibits a clear core-shell structure in which the particles near the wall sediment with velocities close to the mean, whereas the particles in the core sediment at either much faster or much slower velocities. This seems to happen in large vertical structures, specifically at $t = t_{dev}$.

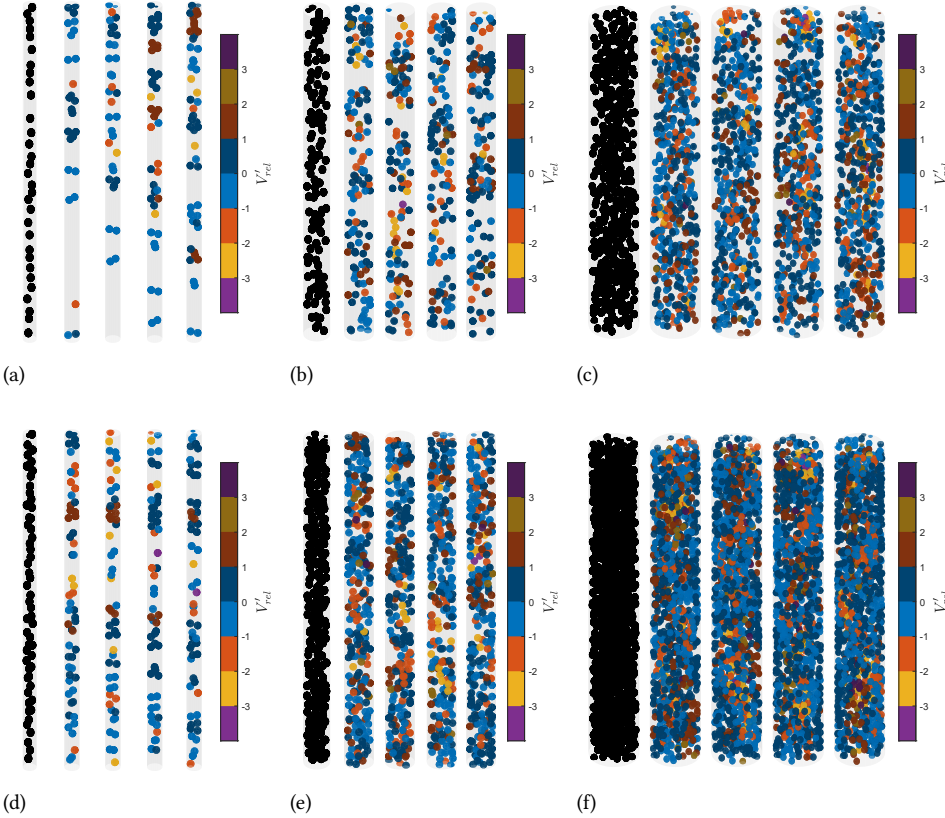


Figure 2.3: Instantaneous particle positions for the cases with (a) $D/d = 2$, (b) $D/d = 4$, and (c) $D/d = 8$ for a volume concentration of $\phi_b = 0.1$, and (d) $D/d = 2$, (e) $D/d = 4$, and (f) $D/d = 8$ for a volume concentration of $\phi_b = 0.2$ at five different time instants from left to right corresponding to $t = 0$, $t = 0.25t_{dev}$, $t = 0.5t_{dev}$, $t = 0.75t_{dev}$, and $t = t_{dev}$, respectively. Colors show the relative velocity fluctuations $V'_{rel} = (V - V_{mean})/V_{rms}$, where negative values indicate particles settling faster than the average settling velocity. The black color for $t = 0$ represents the initial condition, where particles have zero velocity.

The **relative velocity fluctuations**, visualized by the colors in Figure 2.3, have been

quantified by determining the probability density function (PDF), as shown in Figure 2.4. The PDF of the cases with $D/d = 2$ is not smooth, which is likely due to a lack of statistical sampling in these cases. Nevertheless, 3 distinct peaks can clearly be observed, of which 2 large ones are close to the mean and 1 smaller one corresponds to particles falling much faster than the mean. The sharp peak in between $V'_{rel} = -1$ and 0 and the small peak in between $V'_{rel} = -3$ and -2 for $D/d = 2$ in Figure 2.4a appear to be related to, respectively, the bright-blue colored particle doublets and the bright-yellow colored isolated particles in Figure 2.3a. Interestingly, most particle doublets settle predominantly with a horizontal orientation, which suggests that a vertical orientation is unstable. For the larger diameter ratios, the PDF appears much smoother, a confirmation of statistical convergence. A distinct difference is visible between the two bulk volume fractions, where the PDF for $\phi_b = 0.1$ is negatively skewed with the peak at $V'_{rel} \approx 0.5$ (particles falling somewhat slower than the mean) and a long tail towards negative values of V'_{rel} (particles falling much faster than the mean). The shape of the curve is the same for all diameter ratios of $D/d \geq 4$. The skewed PDF is a sign of particle clustering and shows similarities to the PDF found for unbounded sedimentation of dilute suspensions in the inertial regime at high Ga [7, 25]; in fact, this is a strong indication that the skewness originates from the previously observed preferential alignment in the vertical direction and the presence of vertical particle trains in Figure 2.3b. In contrast, the PDF for $\phi_b = 0.2$ is symmetric and has a super-Gaussian shape. Additionally, the PDF is dependent on the diameter ratio, with increasing peak height for larger D/d . This increase in peak height and corresponding lengthening of the tails seems to indicate collective movement of the majority of particles in rather stable clusters, based on the similarity with the super-Gaussian PDF for *horizontal* velocity fluctuations for unbounded sedimentation of moderately dense suspensions in the inertial regime [7]. This is confirmed by Figure 2.3, which shows an increase in collective movement and cluster size with increasing tube diameter for $\phi_b = 0.2$.

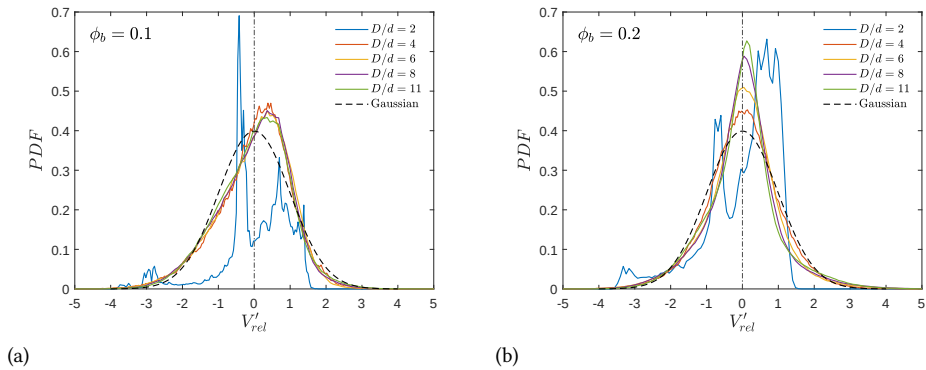


Figure 2.4: Probability density function (PDF) of the vertical velocity fluctuations $V'_{rel} = (V - V_{mean})/V_{rms}$, calculated for the steady state of the simulations. Negative values of V'_{rel} indicate particles settling faster than the average settling velocity.

The **particle-averaged velocity** in the steady state was used to determine the mean

sedimentation velocity, V_s , of the suspensions by averaging over time. This sedimentation velocity shows good agreement with the correlation developed by Richardson and Zaki [9], Equation (2.5). Figure 2.5 shows the natural logarithm of the sedimentation velocity normalized by the Stokes velocity, $\ln(|V_s|/V_{St})$, as a function of the natural logarithm of the void fraction, $\ln(1 - \phi_b)$. The dashed lines show the Richardson and Zaki correlation fitted to the DNS data. The slope of the fits corresponds to the exponent, n , in the Richardson and Zaki correlation. The intercept of the fits with the line $\ln(1 - \phi_b) = 0$ yields a proxy for the terminal settling velocity of a single particle, $V_{s, \phi_b \rightarrow 0}$. To determine the prefactor, k , in the Richardson and Zaki correlation, we first replaced the velocity V_0 for an unbounded domain in Equation (2.5) by V_T for a bounded domain. Next, k was computed from $k = V_{s, \phi_b \rightarrow 0}/V_T$. The actual terminal settling velocity for a single particle, V_T , is indicated by the black markers in Figure 2.5. The values we found for n and k are shown in Figures 2.6a and 2.6b, respectively. Figure 2.6a shows that n is approximately 4.1 for the cases with $D/d = 4$ to 11, indicating that the scaling of the sedimentation velocity with volume fraction is not strongly affected by the diameter ratio for the range investigated here. In contrast, the case with $D/d = 2$ shows a distinct difference where $n \approx 1$. Comparing this to the correlations and values from literature shows that our data for $D/d \geq 4$ is very close to the value found by Yin and Koch [51]. The correlations proposed by Richardson and Zaki [9], Equations (2.7a) and (2.7b), show values that are much larger and diverge from our findings with decreasing D/d . Equation (2.8b) is closer to our results, but still overestimates the value of n and doesn't capture the decrease in n for $D/d = 2$. From Figure 2.6b we observe that $k \approx 0.78$ for $D/d \geq 6$, which is very close to the value of 0.8 reported by Di Felice and Parodi [28]. For the case with $D/d = 4$, we see a slight deviation to a smaller value of $k = 0.73$, whereas the deviation is larger with a value of $k = 0.4$ for the case with $D/d = 2$. This deviation indicates that the dynamics are different for the case with $D/d = 2$ and that there appears to be a transition around $D/d = 4$. The relation proposed by Garside and Al-Dibouni [26], Equation (2.8a), gives a reasonable description of our data; however, the plateau around $k = 0.78$ starts at smaller D/d than is captured by the correlation. The correlations by Francis [13] and Di Felice [71] show a stronger decrease of k at small D/d , underestimating the value for k up to $D/d \approx 10$.

From the results shown in Figure 2.6, we can conclude that the coefficients in the modified Richardson and Zaki correlation, n and k , are only affected by confinement for very small D/d ratios. Based on this and the earlier observation that the Francis correlation accurately captures the effect of confinement for a single settling particle, we propose the following modified correlation for the sedimentation velocity in a vertical tube:

$$V_s = kV_0(1 - \phi_b)^n \left(\frac{1 - \lambda}{1 - 0.475\lambda} \right)^4, \quad (2.14)$$

where $V_0 \approx -0.96V_{St}$, $n \approx 4.12$ for $D/d \geq 4$, and $k \approx 0.78$ for $D/d \geq 6$ in the present study. The finding that n and k are constant, indicates that the effect of confinement appears only as a wall effect on the velocity of a single settling particle for $D/d \geq 6$. Figure 2.7 shows the mean sedimentation velocity as a function of the tube-to-particle diameter ratio for all different volume concentrations, including the single particle simulations. The dashed line shows the Francis correlation for the single particle sedimentation, while the solid lines show the model in Equation (2.14) for the different solid volume fractions. This

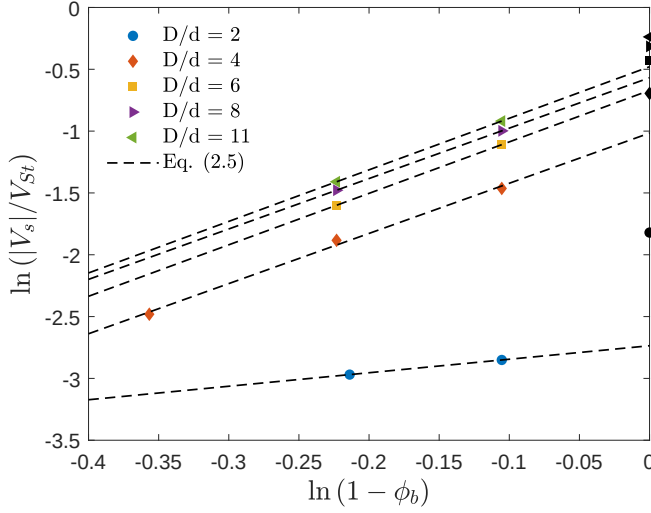


Figure 2.5: Mean sedimentation velocity as a function of the bulk void fraction, $1 - \phi_b$, on double logarithmic scale. Black markers indicate the terminal velocity of a single settling particle.

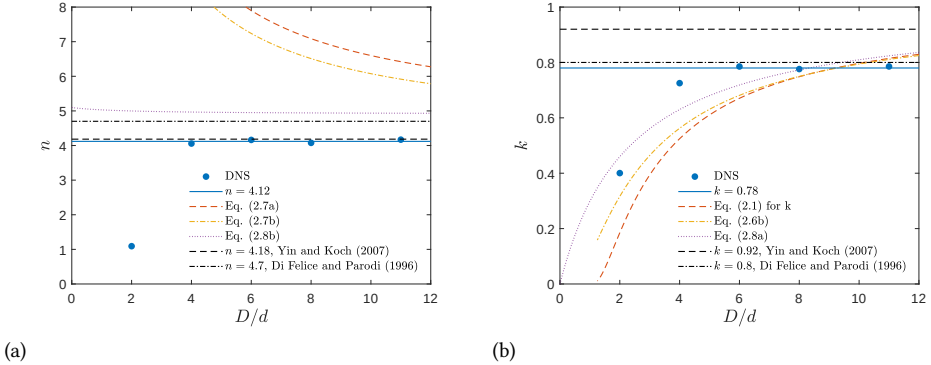


Figure 2.6: Exponent n (a), and prefactor k (b) in the Richardson and Zaki correlation, Equation (2.5) with V_0 replaced by V_T for the DNS data, as a function of the tube-to-particle diameter ratio D/d . Markers indicate the values obtained from our DNS simulations, with the solid line indicating the plateau, and the dashed lines show models and findings from literature.

clearly shows that the sedimentation velocity increases with increasing diameter ratio for all concentrations. The increase in velocity levels off towards larger diameter ratio. Based on Equation (2.14), for tube diameters larger than 20.8 particle diameters ($\lambda < 0.048$), the effect of confinement on the sedimentation velocity is less than a 10% reduction. Additionally, the sedimentation velocity is higher for a lower solid volume concentration. This difference seems to get smaller with decreasing diameter ratio and is almost absent for

$D/d = 2$, suggesting that the effect of confinement is dominant over the effect of particle concentration in this very narrow tube. The modified hindered settling equation captures both the effect of confinement and the effect of concentration on the sedimentation velocity very well. It is worthwhile to mention that the trends we observe do not always seem to hold. For example, in the experiments of Heitkam et al. [72], stabilization of convection structures causes the mean sedimentation velocity for a suspension in a narrow tube to exceed the Stokes velocity under certain conditions. This effect is said to occur at very low Reynolds number and is strongest in capillaries of diameters from 5 to 20 times $d\phi_b^{-1/3}$. We did not expect to observe this phenomenon in our simulations, due to the higher Reynolds number and smaller tube diameters considered in our study.

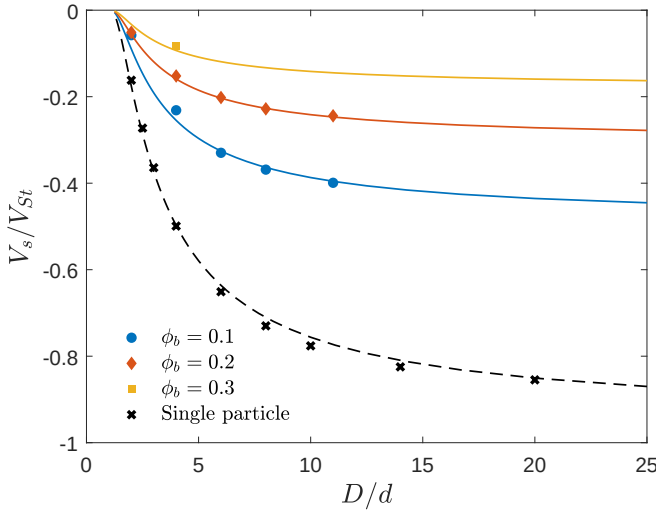


Figure 2.7: Mean sedimentation velocity as a function of tube-to-particle diameter ratio (D/d), using $V_0 = -0.96V_{St}$, $n = 4.12$, and $k = 0.78$. The solid lines show the modified correlation for the sedimentation velocity, Equation (2.14). The dashed line shows the Francis correlation, Equation (2.1), for a single settling particle.

In the following, we take a closer look at the **particle velocity fluctuations** to gain further insight into the particle dynamics. Figure 2.8a shows the root-mean-square (rms) of the vertical particle velocity normalized by the mean sedimentation velocity and shown as a function of $D/(d\phi_b^{-1/3})$. Interestingly, for sufficiently large tube diameters, the data can be described by a correlation of the form $0.28\phi_b^{1/3}(D/d)^{2/3}$, shown by the solid lines. For the smaller tube diameters, a change in scaling is observed, and the rms velocity appears to scale with $0.52\phi_b^{1/9}$, indicating a difference in dynamics for small tubes with $D \lesssim 2.5d\phi_b^{-1/3}$. If we now normalize the rms velocity by $\phi_b^{1/3}(D/d)^{2/3}$, as is shown in Figure 2.8b, it becomes clear that this scaling holds for the rms in all three directions when a different pre-factor is applied. The magnitude of the rms is larger in the vertical direction compared to the radial and azimuthal directions. Furthermore, we can clearly see that the deviation for small tube diameter ratios starts at $D \lesssim 2.5d\phi_b^{-1/3}$.

We also studied the temporal autocorrelation of the particle velocity fluctuations in

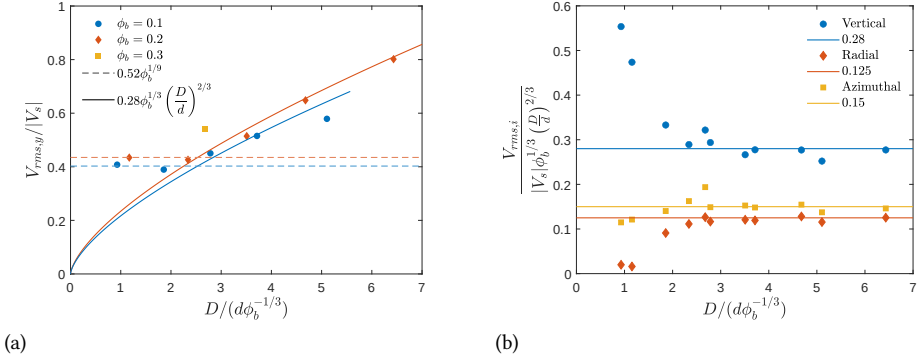


Figure 2.8: (a) rms of the vertical particle velocity normalized by the mean sedimentation velocity and (b) scaled rms of the velocity fluctuations for all directions, as a function of $D/(d\phi_b^{-1/3})$.

the vertical (y), radial (r), and azimuthal (θ) directions. The autocorrelation is defined as:

$$\rho_i(\tau) = \frac{\overline{(V_i(t) - V_{m,i})(V_i(t + \tau) - V_{m,i})}}{\overline{(V_i(t) - V_{m,i})^2}}, \quad (2.15)$$

where V_i denotes the velocity in direction i , $V_{m,i}$ the mean particle velocity in direction i , and the averaging is done over time and all particles in the system. Figure 2.9a shows the autocorrelation for the vertical direction, where the lag time, τ , is normalized by the Stokes time, t_{St} . This figure shows that the correlation is dependent on the bulk volume fraction, with faster decorrelation for higher solid volume fraction. Furthermore, for $\phi_b = 0.1$ (solid lines), the dependency on the tube diameter is visible, with faster decorrelation for larger tube diameter. On the contrary, for $\phi_b = 0.2$, the influence of tube diameter appears negligible for $D/d \geq 4$. Also, the results for $\phi_b = 0.2$ (excluding the case with $D/d = 2$) and $\phi_b = 0.3$ nearly collapse, indicating a difference in sedimentation dynamics between the low ($\phi_b = 0.1$) and higher concentrations ($\phi_b = 0.2$ and 0.3). Figure 2.9b shows a pretty good collapse of the data when scaling the lag time with τ_y , where τ_y is defined by:

$$\tau_y = \frac{D\phi_b^{-1}}{V_{rms,y}}. \quad (2.16a)$$

Figures 2.9c and 2.9d show the temporal correlation for the radial velocity component, with the time lag time normalized by, respectively, t_{St} and τ_r defined as:

$$\tau_r = \frac{D\phi_b^{-1/3}}{V_{rms,r}}. \quad (2.16b)$$

Interesting, both normalizations of the lag time yield a similar collapse of the correlation profiles for $D/d \geq 4$, indicating that τ_r/t_{St} is approximately constant in this range. Finally, Figures 2.9e and 2.9f show the temporal correlation for the azimuthal velocity component,

with the time lag time normalized by, respectively, t_{St} and τ_θ defined as:

$$\tau_\theta = \frac{D^{2/3} d^{1/3} \phi_b^{-1/3}}{V_{rms,\theta}}. \quad (2.16c)$$

For $D/d \geq 4$, the normalization of the time lag with τ_θ yields clearly a better collapse of the correlation than when using t_{St} . The opposite is true for $D/d = 2$, where normalization with t_{St} yields an almost perfect collapse of the two profiles for lag times up to $\approx 50t_{St}$. For all three coordinate directions, the correlations for $D/d = 2$ strongly deviate from the correlations for $D/d \geq 4$, indicating a clear difference in the sedimentation dynamics.

From the particle rms velocities and temporal autocorrelations, the particle diffusivities can be computed according to $\mathcal{D}_i = 2V_{rms,i}^2 \mathcal{T}_i$ with $\mathcal{T}_i = \int_0^\infty \rho_i(\tau) d\tau$ the integral timescale [7, 73, 74]. This has been used to define a Lagrangian lengthscale of correlated particle motions according to $\mathcal{L}_i = \mathcal{D}_i / V_{rms,i} = 2V_{rms,i} \mathcal{T}_i$. The result is shown in Figure 2.10, as a function of $D/(d\phi_b^{-1/3})$. Note that the Lagrangian lengthscale is normalized with $V_{rms,i} \tau_i$. The data shows a plateau for $D/(d\phi_b^{-1/3}) \gtrsim 2.5$ with the following scaling relations for the vertical, radial, and azimuthal directions, respectively:

$$\mathcal{L}_y \approx 0.091 D \phi_b^{-1}, \quad (2.17a)$$

$$\mathcal{L}_r \approx 0.009 D \phi_b^{-1/3}, \quad (2.17b)$$

$$\mathcal{L}_\theta \approx 0.019 D^{2/3} d^{1/3} \phi_b^{-1/3}. \quad (2.17c)$$

The constants are determined by the best fit to the data for $D/(d\phi_b^{-1/3}) > 2.5$. It is interesting to note that the Lagrangian lengthscales in the axial and the radial direction do solely depend on the tube diameter and the concentration, while there is also a weak dependence on the particle diameter in the azimuthal direction. The typical lengthscale of correlated particle motions is thus primarily controlled by the tube diameter, as expected for the small tube diameters considered in the present study. Interestingly, while $\mathcal{L}_r$ and $\mathcal{L}_\theta$ are of comparable magnitude, $\mathcal{L}_y$ appears much larger for the parameter ranges considered in the present study. Based on Equations (2.17a) and (2.17b) and for the range of $D/(d\phi_b^{-1/3}) > 2.5$, the ratio $\mathcal{L}_y/\mathcal{L}_r$ varies from ≈ 17 (for $D/d = 4$ and $\phi_b = 0.3$) to ≈ 49 ($D/d = 11$ and $\phi_b = 0.1$). This indicates the presence of vertically elongated structures of correlated particle motions, consistent with the preferential alignment of particles in the vertical direction as previously discussed after Figure 2.3.

To gain additional insight in the particle dynamics, we also analyzed the **temporal development of the spatial particle distribution** within the pipe along the vertical direction. To this purpose, we computed the spatiotemporal evolution of the horizontal plane average particle concentration, $\phi_{local}(y, t)$. Figure 2.11 shows the plane-averaged concentration as a function of height and time for all cases considered, where $t/t_{St} = 0$ denotes the start of the simulation with an initially random particle distribution. The color shows the local volume concentration normalized by the bulk volume concentration, where the dark brown and dark blue spots show clusters and voids respectively. The black dashed lines indicate the mean sedimentation velocity. Starting at the smallest diameter ratio of $D/d = 2$, the figures show that there is a strong tendency to form persistent clusters that

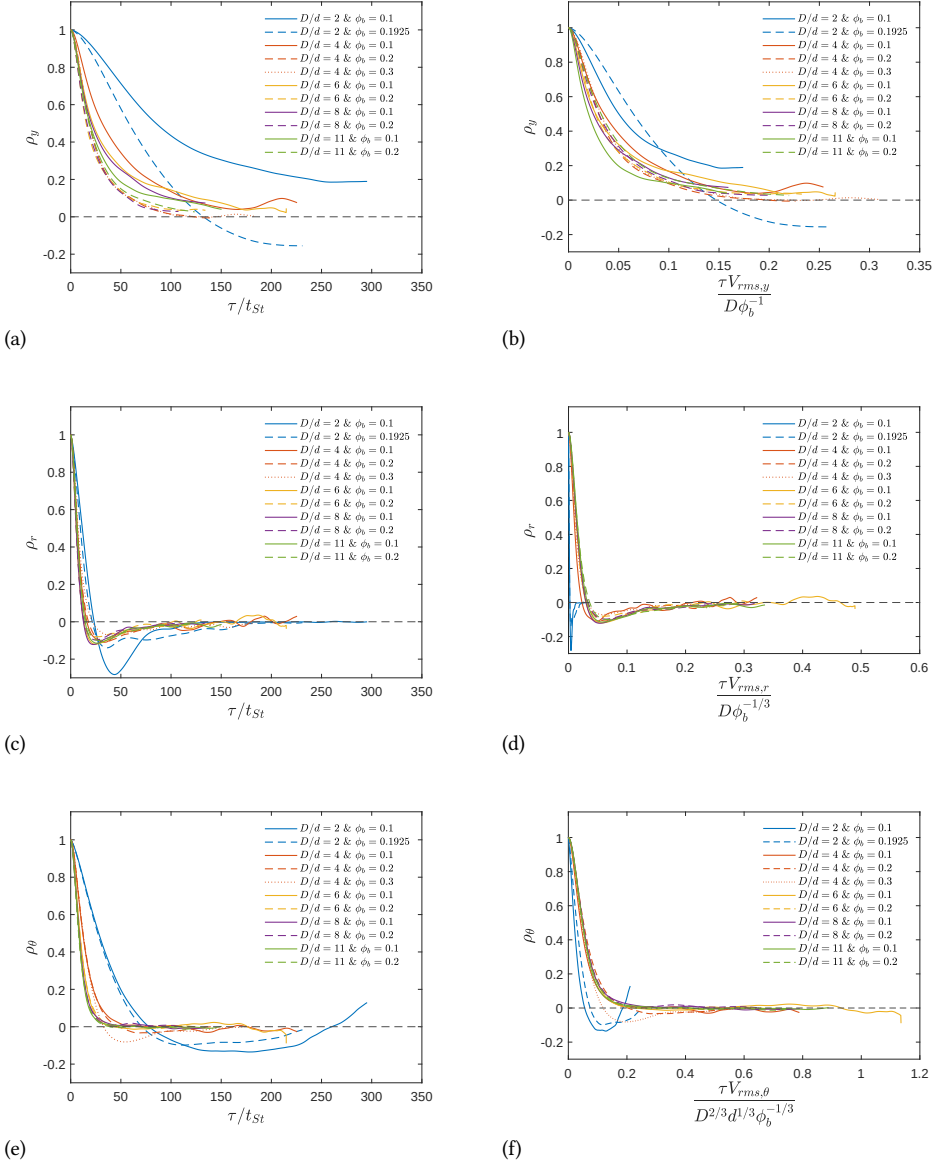


Figure 2.9: Temporal autocorrelation of velocity fluctuations in the vertical (a,b), radial (c,d), and azimuthal (e,f) directions. Note the difference in normalization of the time lag.

can be seen from the dark brown streaks. Between the clusters, the blue areas show that there are voids in the domain where no particles are present. The downward propagation of the clusters is slower than the mean sedimentation velocity, which can be seen by

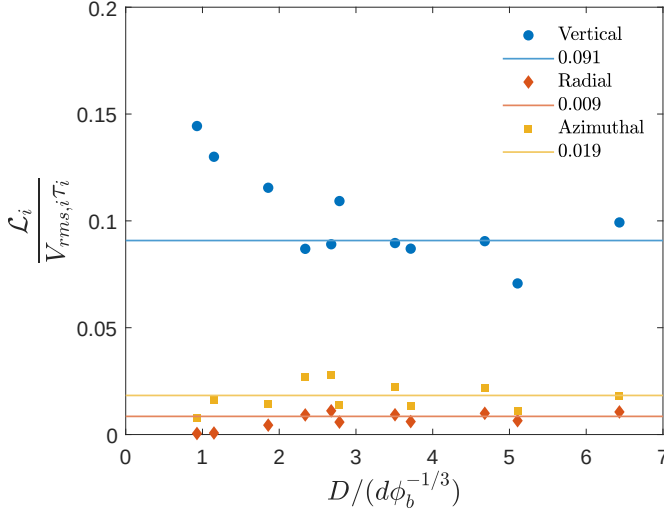


Figure 2.10: Normalized Lagrangian lengthscale as a function of $D/(d\phi_b^{-1/3})$. Lines indicate the best fit to the data for $D/(d\phi_b^{-1/3}) > 2.5$.

comparing the slope of the dark brown streaks to the slope of the black dashed line. The clustering seems to change from a small number of relatively large clusters to a larger number of clusters with increasing bulk volume concentration. The cases with $D/d = 4$ show less distinct clustering, however, the continuous streaks indicate that the clusters exist for extended periods of time. Propagation of the clusters is not solely downwards for these cases, as the streaks have a positive slope for the higher bulk volume fractions, $\phi_b = 0.2$ and 0.3 . This does not mean that particles move upwards, but that there is a supply of faster falling particles from the top and a loss of particles at the bottom of a cluster. This behavior is consistent with the presence of the vertically propagating kinematic waves, a well-known feature of sedimenting suspensions both in the viscous and in the inertial regime and related to the concentration-dependent sedimentation velocity [75, 7]. In general, we can say that when the diameter ratio and/or the bulk concentration are increased, the tendency for clustering decreases, possibly caused by enhanced dispersive damping of kinematic waves at the higher concentrations originating from short-range multiparticle interactions [7]. This is clearly visible in the decrease of dark brown streaks; however, clusters are still present but seem less persistent. Meaning that the clusters form, but also break up within the timespan of the simulations. As mentioned before, a long transient is visible for the case with $D/d = 2$ and $\phi_b = 0.05$, which is longer than the extent of the simulation, exemplifying why this case was not taken into account for the calculation of steady-state statistics.

In order to investigate whether the behavior of particles in clusters is determined by the local volume fraction or the tube-to-particle diameter ratio, the **conditionally averaged vertical velocity** has been calculated as a function of the local plane-averaged concentration. The result is shown in Figure 2.12. The left column shows V/V_s as a func-

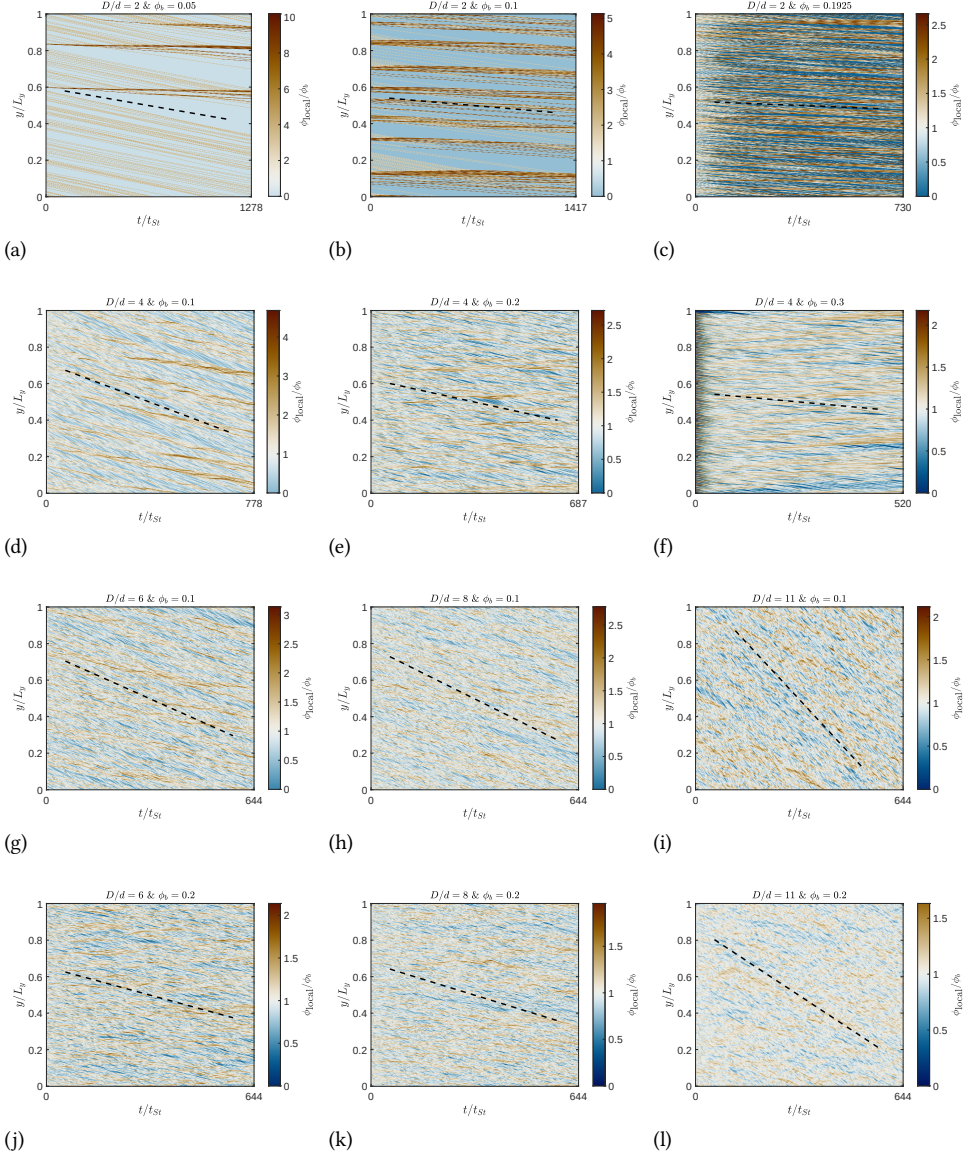


Figure 2.11: Height-time plot of the horizontal plane average particle concentration for all cases considered. Color shows the local volume fraction normalized by the bulk volume fraction. Black dashed line indicates the mean sedimentation velocity. Subfigures (a,b,c) show $D/d = 2$, (d,e,f) show $D/d = 4$, (g,j) show $D/d = 6$, (h,k) show $D/d = 8$, and (i,l) show $D/d = 11$.

tion of ϕ_{local} , while the right column shows the same data but zoomed in the range of $V/V_s \in [0.8 : 1.3]$ and with the local concentration normalised by the bulk concentration,

ϕ_{local}/ϕ_b . The datapoints at the left and right ends of the series that strongly deviate from the trend are prone to larger statistical uncertainty, as these local volume fractions are less frequent. Looking at the right column we observe that for $D/d = 2$ the settling velocity decreases with increasing ϕ_{local}/ϕ_b for $\phi_{local}/\phi_b \gtrsim 1$. For $D/d = 4$, the dependence of the velocity on the local volume fraction seems to change with bulk volume fraction. At a bulk volume fraction of $\phi_b = 0.1$, the velocity increases slightly towards high local volume fraction, whereas the velocity increases towards low local volume fraction for $\phi_b = 0.2$ and 0.3 . In contrast, for $D/d \geq 6$, the settling velocity only has a very weak dependence on the local volume fraction. This weak dependence seems to contradict the findings from Figure 2.11, where streaks or wave-like patterns are observed travelling at velocities different from the mean sedimentation velocity. However, as indicated earlier, the propagation velocity of these streaks does not correspond to the particle velocity within these streaks. Furthermore, the nearly constant vertical velocity seems consistent with the aforementioned loss of spatiotemporal coherence of the streaks for the larger tube diameters and higher concentrations.

Figure 2.12 also provides information about the density of the clusters that are visible in Figure 2.11. The highest local volume fraction present in the suspensions is at least 1.5 times higher than the bulk concentration for all cases. For the cases with $D/d = 2$, the maximum in ϕ_{local} seems independent of the bulk volume fraction, which indicates that the clustering is governed by the diameter ratio for this narrow tube. For the wider tubes, the maximum local volume fraction is dependent on the bulk concentration, indicating that the cluster density is not solely dependent on the diameter ratio. It is interesting to note that the range of local volume fractions observed in the system becomes smaller for increasing diameter ratio until $D/d \geq 8$ for which the range stays the same.

To assess the heterogeneity of the **particle distribution in the radial direction**, we computed the mean radial position of the particles at statistically steady state. This is plotted in Figure 2.13. The dashed line indicates the expected mean radial position for a homogeneous particle distribution, $\bar{r}/((D-d)/2) = 2/3$. Comparing the mean positions to the expected position for a homogeneous distribution shows that the particles are closer to the wall for all cases. The mean radial position becomes closer to that for a homogeneous distribution for larger D/d . This figure shows that the mean radial position of the particles decreases with larger diameter ratio. Additionally, the effect of the volume concentration seems to be small; however, the effect of the solid volume concentration seems to increase slightly with increasing diameter ratio. At $D/d = 2$, the particles appear to be touching the tube wall, according to the mean radial position of $\bar{r}/((D-d)/2) \approx 1$. This is probably caused by the formation of clusters within which particles tend to align horizontally and the limited space in the radial direction leads to a large number of particles touching the wall.

Next to the mean radial position, the radial distribution of the particles was analyzed. This is done by calculating the number fraction of particles within a certain radial position, which was then normalized by the expected number fraction for a homogeneous suspension. The radial distribution of particles is shown in Figure 2.14, where $(R-r)/d$ shows the distance from the tube wall in particle diameters. The data is grouped by the tube-to-particle diameter ratio, with increasing ratio from top to bottom. Note that the y-axis is on a logarithmic scale for all cases and has a larger extent for the cases with $D/d = 2$. This

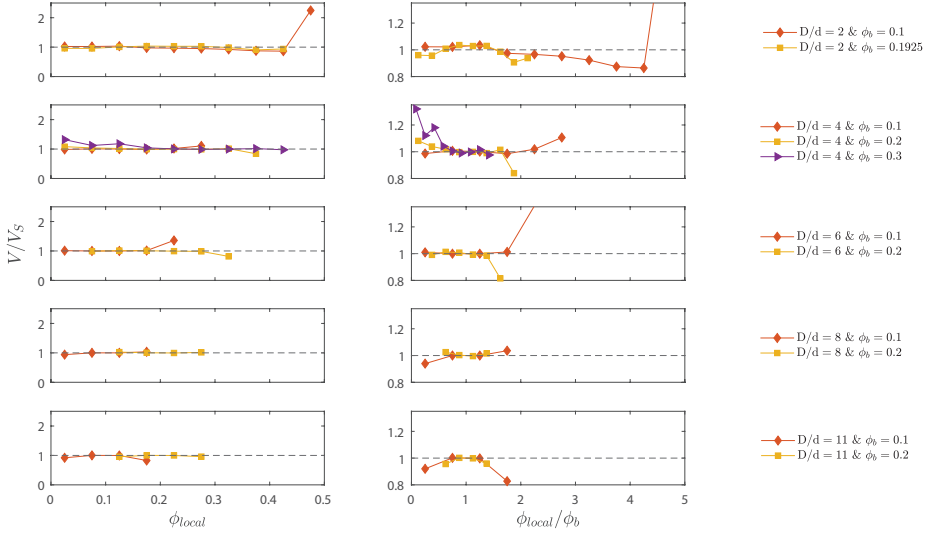


Figure 2.12: Particle velocity normalized by the mean sedimentation velocity as a function of the horizontal plane average particle concentration. Data is grouped by tube-to-particle diameter ratio, which is increasing from top to bottom.

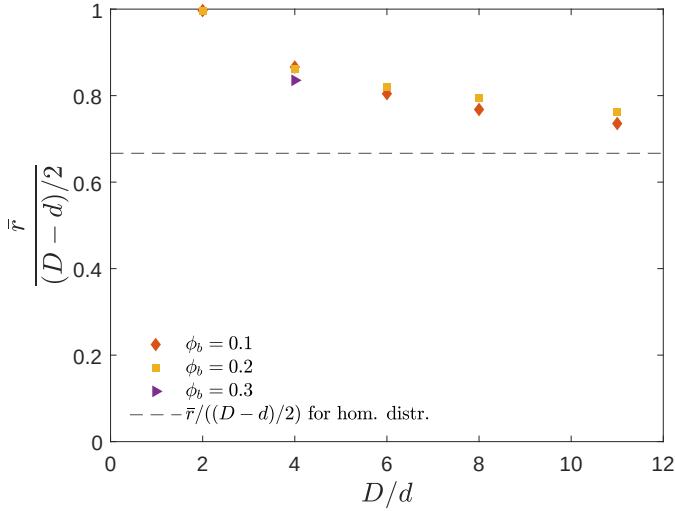


Figure 2.13: Mean radial particle position as a function of the tube-to-particle diameter ratio and bulk solid volume fraction. The dashed line shows the expected mean radial position for a homogeneous distribution of particles at $\bar{r}/((D-d)/2) = 2/3$.

figure shows the change in distribution that causes the change in mean radial position that was observed in Figure 2.13. The radial distribution of all cases shows a peak near the tube wall ($(R-r)/d = 0.5$ as this is based on the particle centroid and particles cannot overlap with the wall), meaning that there is a larger fraction of particles at the tube wall than is expected for a homogeneous distribution. This is indicative of preferential alignment of particles along the tube wall, which can also be observed from Figure 2.3 after close inspection. The radial distribution of particles becomes closer to that of a homogeneous suspension with increasing diameter ratio, as was also observed in the mean radial position. However, there is still a large difference close to the wall, where particles appear to accumulate.

Looking closer at the individual cases, there are some interesting results to note. The cases with $D/d = 2$ show a decreasing particle fraction towards the core, which even vanishes for values of $(R-r)/d < 1$. This indicates that there are no particles near the centerline of the tube. The cases with $D/d = 4$ show an additional peak at a radial position of $(R-r)/d \approx 1.4$, which is stronger for a higher bulk volume fraction. The radial position of this peak is slightly higher than the secondary peak of $(R-r)/d = 0.5(1 + \sqrt{8/3}) \approx 1.3$ for a hexagonal close packing of spheres. This internal peak in the concentration is also observed for larger D/d , but becomes less sensitive to the bulk concentration. In addition, the difference between the concentration in the tube core and the internal peak concentration diminishes for increasing D/d values. A similar observation holds for the local minimum in the concentration in between the internal concentration peak and the concentration peak at the wall: the local minimum becomes less distinct, although it remains dependent on the bulk concentration. To conclude, from these distributions it becomes clear that the radial distribution of particles is not homogeneous, with the presence of two distinct peaks in the concentration near the wall. For increasing D/d , there is a tendency towards a more homogeneous distribution but with the exception of near-wall region, where particle alignment along the wall and related concentration peaks are expected to remain present. The latter is also referred to as an ‘excluded volume effect’ in literature [56], originating from the constraint that particles cannot overlap with the tube wall and hence tend to align themselves along the wall, which changes the local suspension microstructure with respect to the core region far away from the wall.

In a similar way, we computed the **vertical particle velocity as a function of the radial position** of the particles, as is shown in Figure 2.15. The velocity is normalized by the mean sedimentation velocity, in order to make a fair comparison between the cases. For $D/d = 2$, the particles close to the wall, where the concentration has a large peak, move approximately at the mean sedimentation velocity. For $D/d = 4$ and $\phi_b = 0.1$, the velocity profile is uniform over almost the entire tube and higher than the mean velocity, while the concentrated layer of particles close to the wall moves significantly slower. Interestingly, at $D/d = 4$, a change in the velocity profile is observed for $\phi_b = 0.2$ and 0.3 as compared to $\phi_b = 0.1$: a local velocity maximum is present centered around $(R-r)/d \approx 1.4$, while the velocity near the centerline and in the wall region is close to the mean sedimentation velocity. This local maximum occurs at the observed interior concentration peak for $D/d = 4$ in Figure 2.14, and which is more pronounced for $\phi_b = 0.2$ and 0.3 as compared to $\phi_b = 0.1$. For the cases with $D/d \geq 6$, there is also a clear distinction between $\phi_b = 0.1$ and 0.2 . The cases with $\phi_b = 0.1$ show a velocity approximately equal to the mean sedimentation velocity for

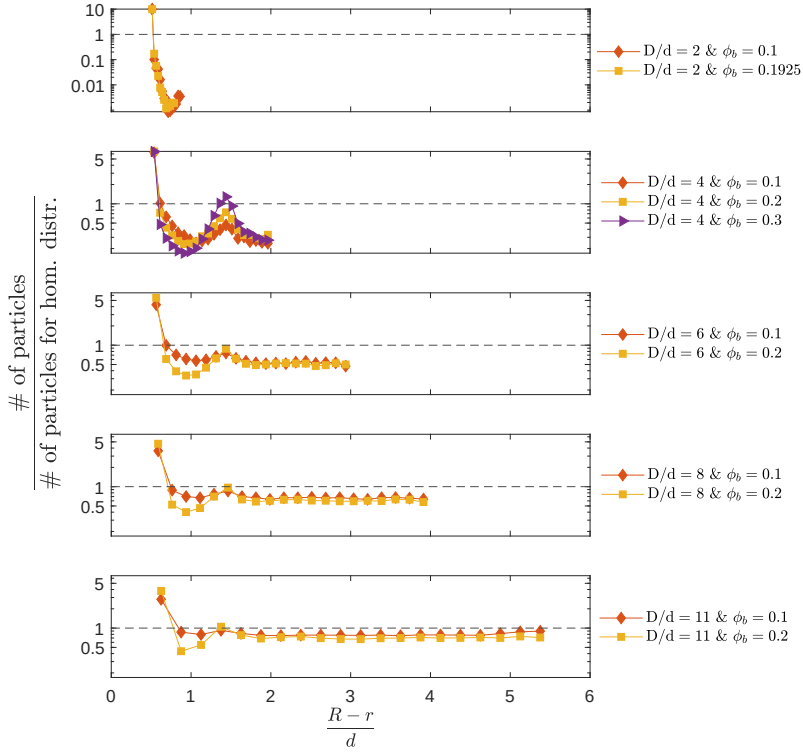


Figure 2.14: Radial distribution of particles normalized by the expected radial distribution for a homogeneous suspension, where $(R-r)/d$ shows the distance from the tube wall in particle diameters. Data is grouped by the tube-to-particle diameter ratio, which is increasing from top to bottom. Note that the y-axis is on a logarithmic scale for all cases and has a larger extent for the cases with $D/d = 2$.

the core region of the tube and the velocity decreases sharply near the wall. On the contrary, the cases with $\phi_b = 0.2$, have a velocity lower than the mean in the core region, with a gradual increase to a maximum larger than the sedimentation velocity at $(R-r)/d \approx 1.4$, followed by a decrease to a local minimum near the tube wall. It is interesting to note that this peak in velocity again, just as for $D/d = 4$, corresponds to the internal concentration peak for these cases as observed in Figure 2.13. The velocity profiles for $\phi_b = 0.2$ cannot be explained by the intrinsic convection pattern found for dilute sedimenting suspensions as discussed in the introduction, since (a) the velocity has a minimum in the core, and (b) the local concentration largely exceeds the bulk concentration near the wall in our simulations; the latter is consistent with the observation of concentrated particle-wall layers in the experiments of Peysson and Guazzelli [60]. We speculate that the observed velocity profile for $\phi_b = 0.2$ is related to the presence of concentrated particle clusters around the internal concentration peak, which causes a rather stable streaming-like pattern as also were observed in, e.g., polydisperse suspensions consisting of a bidisperse mixture

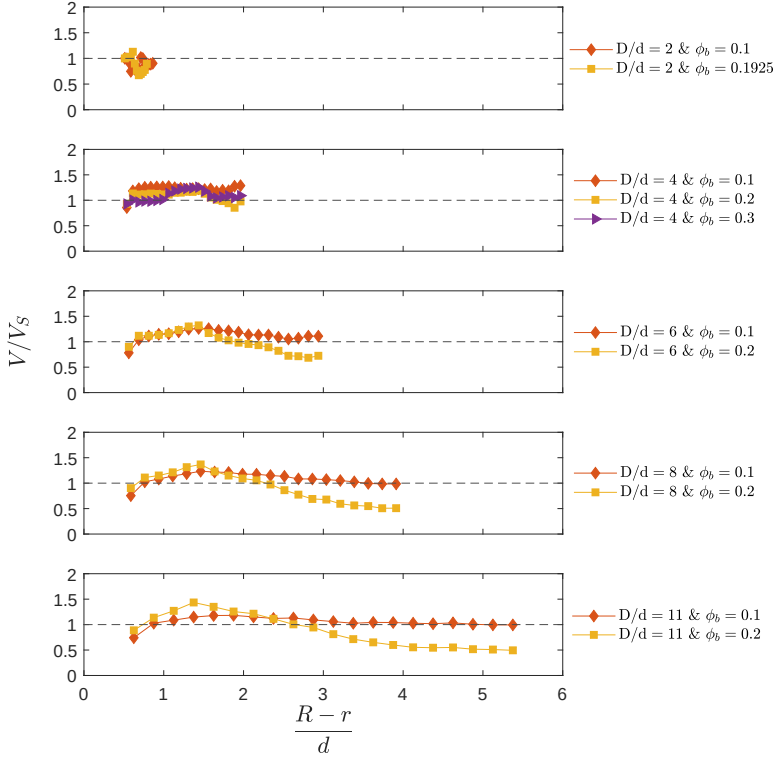


Figure 2.15: Particle velocity as a function of radial position, where $(R-r)/d$ shows the distance from the tube wall in particle diameters. Data is grouped by tube-to-particle diameter ratio, which is increasing from top to bottom.

of heavy and light particles (heavy streams that are falling faster, lighter streams that are falling slower than the average sedimentation velocity). The rather stable streaming pattern might explain the super-Gaussian behavior of the PDF for $\phi_b = 0.2$ as observed before in Figure 2.4.

2.5 Conclusions

We performed particle-resolved Direct Numerical Simulations to gain understanding of the influence of confinement on sedimentation of dense particle suspensions in narrow vertical tubes in the viscous flow regime. The Galileo number used in this study was $Ga = \sqrt{18}$, corresponding to a Reynolds number $V_{St}d/\nu_f = 1$ based on the Stokes velocity. The range of tube-to-particle diameter ratios studied is $D/d = 2$ to 11, while the bulk solid volume concentration was varied from $\phi_b = 0.05$ to 0.3. The sedimentation dynamics was analyzed in terms of particle statistics, including the mean and rms particle velocities, temporal particle velocity correlations, particle clustering in the vertical direction, and

the radial particle concentration and particle velocity distributions. With these statistics we obtained both a clear picture of the macroscopic suspension behavior as well as insight in the underlying suspension microstructure.

Single particle simulations showed that the effect of D/d can be described very well using the Francis correlation [13]. This indicates that, due to the retarding effect of the tube wall on the sedimentation, the Reynolds number is decreased to a value well within the Stokes regime.

The effect of the volume concentration on the **mean sedimentation velocity** is described well by the Richardson and Zaki correlation [9], but modified to include a prefactor k and replacing the terminal velocity of a single settling particle in free space by the Francis correlation [13]. We found $k \approx 0.78$, close to $k = 0.8$ experimentally determined by Di Felice and Parodi [28]. Furthermore, we found $n \approx 4.12$ for the exponent of the hindered settling function, which matches well with the value of $n \approx 4.2$ reported by Yin and Koch [51] for their case with $Ga = \sqrt{20.8}$. It is worth mentioning that the mean sedimentation velocity is smaller for smaller D/d and larger ϕ_b . Thus, no evidence is found for possible enhanced settling as observed in the experiments of Heitkam et al. [72].

The **vertical particle velocity fluctuations** exhibit a non-Gaussian behavior, a sign of particle clustering: for $\phi_b = 0.1$, the pdf is negatively skewed, while for $\phi_b = 0.2$ the pdf shows super-Gaussian behavior. For $D/(d\phi_b^{-1/3}) \gtrsim 2.5$, the particle rms velocities scale with $V_s \phi_b^{1/3} (D/d)^{2/3}$. The fluctuations are anisotropic, being significantly stronger in the axial than in the radial and the azimuthal directions. For $D/(d\phi_b^{-1/3}) \lesssim 2.5$, the scaling of the rms velocities is very different, which we attribute to the strong effect of confinement on the particle microstructure in this range.

The **temporal autocorrelations** of the particle velocities show clear scaling behavior with the characteristic correlation times expressed by Equations (2.16a), (2.16b), and (2.16c), for the vertical, radial, and azimuthal directions, respectively. From the rms velocities and the temporal correlations, we determined the Lagrangian lengthscales of correlated particle motions. The axial lengthscale appears to be much larger than the lengthscales in the radial and azimuthal direction and is proportional to $D\phi_b^{-1}$, see Equations (2.17a) to (2.17c). This is indicative for large and vertically elongated structures that are primarily limited in extent by the tube diameter and particle-particle interactions.

We observed **vertical concentration heterogeneity** in horizontal plane averages, which shows that there is a strong tendency for clustering in the narrow tubes. The particle clustering in the vertical direction is reminiscent of vertically travelling kinematic waves, see, e.g. Shajahan and Breugem [7]. The clusters become smaller and less persistent with increasing tube-to-particle diameter ratio, which means that the clusters form and break up over smaller timescales. Our evaluation of the results showed that the dynamics are governed by the local concentration for narrow tubes, while this is not the case for wider tubes. We observed that, for $D/d = 2$, the settling velocity decreases with increasing local volume fraction. For $D/d = 4$, the dependence of the velocity on the local volume fraction seems to change with bulk volume fraction, whereas, for $D/d \geq 6$, the settling velocity only has a very weak dependence on the local volume fraction.

The **radial particle distribution** also shows heterogeneity, where the wall-region shows a concentration peak at a distance of $\approx 0.5d$ from the wall due to particle-wall layering as particles cannot overlap with the wall (excluded volume effect). A second and

weaker concentration peak is present at a distance of $\approx 1.4d$. For $D/d \geq 6$, this is followed by a uniform particle distribution in the core at a concentration significantly below the bulk concentration. The particles around the internal concentration peak appear to settle significantly faster than the particles near the wall and in the core, especially for $\phi_b = 0.2$ and $D/d \geq 6$ for which the pdf of the vertical particle velocity also exhibits super-Gaussian behavior. This is indicative for streaming-like behavior of rather stable and vertically elongated particle clusters, somewhat alike the streaming patterns that have been observed in sedimentation of polydisperse suspensions [5].

We speculate that the enhanced settling of the particles at the location of the internal concentration peak originates both from the higher mixture density with respect to the lighter core and from interparticle shielding from the return flow caused by vertical alignment [76]. For future research it is recommended to explore this in more detail, e.g., through a detailed study of the local particle microstructure. Furthermore, an analysis of the forces acting on the particles may reveal why the particles in the dense particle-wall layer settle less fast than the particles in the internal layer around that second concentration peak. When particle-wall friction appears important, this could be further explored by varying the Coulomb coefficient of sliding friction.

For the entire range of tube-to-particle diameters studied, we observed a profound effect of the tube wall on the sedimentation dynamics. Going down in tube diameter we see a change in sedimentation behavior for $D/d \leq 4$ with respect to the larger tube diameters. The dense suspension at $\phi_b = 0.2$ at the largest tube diameter studied, $D/d = 11$, is still within the strongly confined regime as $D/(0.5d\phi_b^{-1/3}) = 12.9$ is smaller than the characteristic blob size reported in literature for unconfined suspensions. Therefore, for future research it is recommended to explore the transition from strongly confined to unconfined suspension in more detail, and the according change in the suspension dynamics. Finally, it would be interesting to explore the influence of polydispersity in particle size as this is common in applications in practice.

References

- [1] Wouter Peerbooms, Antoine E. D. M. van der Heijden, and Wim-Paul Breugem. Data corresponding to the research: Viscous sedimentation of dense suspensions in narrow vertical tubes. 2026.
- [2] Joost van Lingen. Gradient additive manufacturing of energetics research (gamer). *Netherlands Organisation for Applied Scientific Research*, 2022.
- [3] Alexandra Marnot, Katie Koube, Sungwoo Jang, Naresh Thadhani, Josh Kacher, and Blair Brettmann. Material extrusion additive manufacturing of high particle loaded suspensions: a review of materials, processes and challenges. *Virtual and Physical Prototyping*, 18(1):e2279149, 2023.
- [4] James J Griebler, Alexander S Tappan, Simon A Rogers, Jessica W Kopatz, and Anne M Grillet. Methodology to determine printability criteria of highly concentrated pastes through rheological characterization. *Additive Manufacturing*, 96:104578, 2024.
- [5] Robert H Davis and Andreas Acrivos. Sedimentation of noncolloidal particles at low reynolds numbers. *Annual Review of Fluid Mechanics*, 17(1):91–118, 1985.
- [6] Elisabeth Guazzelli and John Hinch. Fluctuations and instability in sedimentation. *Annual review of fluid mechanics*, 43:97–116, 2011.
- [7] Tariq Shajahan and Wim-Paul Breugem. Inertial effects in sedimenting suspensions of solid spheres in a liquid. *International Journal of Multiphase Flow*, 166:104498, 2023.
- [8] Elisabeth Guazzelli and Jeffrey F Morris. *A physical introduction to suspension dynamics*. Cambridge University Press, 2012.
- [9] JF Richarson and WN Zaki. Sedimentation and fluidisation: Part 1. *Trans. Ins. Chem. Eng*, 31:35–53, 1954.
- [10] E Barnea and J Mizrahi. A generalized approach to the fluid dynamics of particulate systems: Part 1. general correlation for fluidization and sedimentation in solid multiparticle systems. *The Chemical Engineering Journal*, 5(2):171–189, 1973.
- [11] John Happel and Howard Brenner. *Low Reynolds number hydrodynamics: with special applications to particulate media*. Martinus Nijhoff Publishers, 1983.
- [12] Peter M Bungay and Howard Brenner. The motion of a closely-fitting sphere in a fluid-filled tube. *International Journal of Multiphase Flow*, 1(1):25–56, 1973.
- [13] Alfred W Francis. Wall effect in falling ball method for viscosity. *Physics*, 4(11):403–406, 1933.

- [14] MITSUGU IWAOKA and TSUTOMU ISHII. Experimental wall correction factors of single solid spheres in circular cylinders. *Journal of Chemical Engineering of Japan*, 12(3):239–242, 1979.
- [15] Vo Fidleris and RL Whitmore. Experimental determination of the wall effect for spheres falling axially in cylindrical vessels. *British journal of applied physics*, 12(9):490, 1961.
- [16] Roland Clift, John R Grace, and Martin E Weber. *Bubbles, drops, and particles*. Dover Publications, Inc., 1978.
- [17] William L Haberman and Rose M Sayre. Motion of rigid and fluid spheres in stationary and moving liquids inside cylindrical tubes. Technical report, David Taylor Model Basin Washington DC, 1958.
- [18] Madeleine Coutanceau and Patrick Thizon. Wall effect on the bubble behaviour in highly viscous liquids. *Journal of Fluid Mechanics*, 107:339–373, 1981.
- [19] JJJ Higdon and George P Muldowney. Resistance functions for spherical particles, droplets and bubbles in cylindrical tubes. *Journal of Fluid Mechanics*, 298:193–210, 1995.
- [20] M Coutanceau. Sur l'étude expérimentale de l'écoulement engendré par une sphere qui se déplace dans l'axe d'un cylindre au-delà du régime de stokes. *CR Acad. Sci. A*, 274:853–856, 1972.
- [21] RP Chhabra, S Agarwal, and K Chaudhary. A note on wall effect on the terminal falling velocity of a sphere in quiescent newtonian media in cylindrical tubes. *Powder technology*, 129(1-3):53–58, 2003.
- [22] R Di Felice. A relationship for the wall effect on the settling velocity of a sphere at any flow regime. *International Journal of Multiphase Flow*, 22(3):527–533, 1996.
- [23] Takeo Kajishima and Saotshi Takiguchi. Interaction between particle clusters and particle-induced turbulence. *International Journal of Heat and Fluid Flow*, 23(5):639–646, 2002.
- [24] Markus Uhlmann and Todor Doychev. Sedimentation of a dilute suspension of rigid spheres at intermediate galileo numbers: the effect of clustering upon the particle motion. *Journal of fluid mechanics*, 752:310–348, 2014.
- [25] Sander G Huisman, Thomas Barois, Mickaël Bourgoïn, Agathe Chouippe, Todor Doychev, Peter Huck, Carla E Bello Morales, Markus Uhlmann, and Romain Volk. Columnar structure formation of a dilute suspension of settling spherical particles in a quiescent fluid. *Physical Review Fluids*, 1(7):074204, 2016.
- [26] John Garside and Maan R Al-Dibouni. Velocity-voidage relationships for fluidization and sedimentation in solid-liquid systems. *Industrial & engineering chemistry process design and development*, 16(2):206–214, 1977.

- [27] GK Batchelor and JT Green. The determination of the bulk stress in a suspension of spherical particles to order c^2 . *Journal of Fluid Mechanics*, 56(3):401–427, 1972.
- [28] Renzo Di Felice and Enrico Parodi. Wall effects on the sedimentation velocity of suspensions in viscous flow. *AIChE journal*, 42(4):927–931, 1996.
- [29] Penger Tong and Bruce J Ackerson. Analogies between colloidal sedimentation and turbulent convection at high prandtl numbers. *Physical Review E*, 58(6):R6931, 1998.
- [30] Russel E Caflisch and Jonathan HC Luke. Variance in the sedimentation speed of a suspension. *Physics of Fluids*, 28(3):759–760, 1985.
- [31] EJ Hinch. Sedimentation of small particles. In *Disorder and Mixing: Convection, Diffusion and Reaction in Random Materials and Processes*, pages 153–162. Springer, 1988.
- [32] Donald L Koch and ESG Shaqfeh. Screening in sedimenting suspensions. *Journal of fluid mechanics*, 224:275–303, 1991.
- [33] Anthony JC Ladd. Hydrodynamic screening in sedimenting suspensions of non-brownian spheres. *Physical review letters*, 76(8):1392, 1996.
- [34] Anthony JC Ladd. Sedimentation of homogeneous suspensions of non-brownian spheres. *Physics of Fluids*, 9(3):491–499, 1997.
- [35] Hélene Nicolai and Elisabeth Guazzelli. Effect of the vessel size on the hydrodynamic diffusion of sedimenting spheres. *Physics of Fluids*, 7(1):3–5, 1995.
- [36] Laurence Bergougnoux and Élisabeth Guazzelli. Non-Poisson statistics of settling spheres. *Physics of Fluids*, 21(9), 2009.
- [37] Laurence Bergougnoux and Élisabeth Guazzelli. Dilute sedimenting suspensions of spheres at small inertia. *Journal of Fluid Mechanics*, 914:A33, 2021.
- [38] Alejandro Boschan, BL Ocampo, M Annichini, and G Gauthier. Velocity fluctuations and population distribution in clusters of settling particles at low reynolds number. *Physics of Fluids*, 28(6), 2016.
- [39] Elisabeth Guazzelli. Evolution of particle velocity correlations in sedimentation. *Physics of Fluids*, 13(6), 2001.
- [40] AJC Ladd. Effects of container walls on the velocity fluctuations of sedimenting spheres. *Physical review letters*, 88(4):048301, 2002.
- [41] N-Q Nguyen and AJC Ladd. Microstructure in a settling suspension of hard spheres. *Physical Review E—Statistical, Nonlinear, and Soft Matter Physics*, 69(5):050401, 2004.
- [42] PN Segre, Eric Herbolzheimer, and PM Chaikin. Long-range correlations in sedimentation. *Physical Review Letters*, 79(13):2574, 1997.

- [43] JM Ham and GM Homsy. Hindered settling and hydrodynamic dispersion in quiescent sedimenting suspensions. *International journal of multiphase flow*, 14(5):533–546, 1988.
- [44] Michael P Brenner. Screening mechanisms in sedimentation. *Physics of fluids*, 11(4):754–772, 1999.
- [45] Philip N Segre, Fang Liu, Paul Umbanhowar, and David A Weitz. An effective gravitational temperature for sedimentation. *Nature*, 409(6820):594–597, 2001.
- [46] Michael P Brenner and Peter J Mucha. That sinking feeling. *Nature*, 409(6820):569–571, 2001.
- [47] Patrick Snabre, Bernard Pouligny, Cyrille Metayer, and François Nadal. Size segregation and particle velocity fluctuations in settling concentrated suspensions. *Rheologica acta*, 48(8):855–870, 2009.
- [48] Donald L Koch. Hydrodynamic diffusion in dilute sedimenting suspensions at moderate reynolds numbers. *Physics of Fluids A: Fluid Dynamics*, 5(5):1141–1155, 1993.
- [49] E Climent and MR Maxey. Numerical simulations of random suspensions at finite reynolds numbers. *International journal of multiphase flow*, 29(4):579–601, 2003.
- [50] E Kuusela, JM Lahtinen, and T Ala-Nissila. Sedimentation dynamics of spherical particles in confined geometries. *Physical Review E*, 69(6):066310, 2004.
- [51] Xiaolong Yin and Donald L Koch. Hindered settling velocity and microstructure in suspensions of solid spheres with moderate reynolds numbers. *Physics of Fluids*, 19(9):093302, 2007.
- [52] Xiaolong Yin and Donald L Koch. Velocity fluctuations and hydrodynamic diffusion in finite-reynolds-number sedimenting suspensions. *Physics of fluids*, 20(4), 2008.
- [53] R Sungkorn and JJ Derksen. Simulations of dilute sedimenting suspensions at finite-particle reynolds numbers. *Physics of Fluids*, 24(12), 2012.
- [54] Antonio F Fortes, Daniel D Joseph, and Thomas S Lundgren. Nonlinear mechanics of fluidization of beds of spherical particles. *Journal of Fluid Mechanics*, 177:467–483, 1987.
- [55] Anthony JC Ladd. Dynamical simulations of sedimenting spheres. *Physics of Fluids A: Fluid Dynamics*, 5(2):299–310, 1993.
- [56] Elisabeth Guazzelli and Jeffrey F Morris. *A physical introduction to suspension dynamics*, volume 45. Cambridge University Press, 2011.
- [57] CWJ Beenakker and P Mazur. Is sedimentation container-shape dependent? *Phys. Fluids*, 28:3203, 1985.

- [58] P Nozieres. A local coupling between sedimentation and convection: Application to the beenakker-mazur effect. *Physica A: Statistical Mechanics and its Applications*, 147(1-2):219–237, 1987.
- [59] U Geigenmüller and P Mazur. Sedimentation of homogeneous suspensions in finite vessels. *Journal of statistical physics*, 53(1):137–173, 1988.
- [60] Yannick Peysson and Élisabeth Guazzelli. An experimental investigation of the intrinsic convection in a sedimenting suspension. *Physics of Fluids*, 10(1):44–54, 1998.
- [61] D Bruneau, F Feuillebois, R Anthore, and EJ Hinch. Intrinsic convection in a settling suspension. *Physics of Fluids*, 8(8):2236–2238, 1996.
- [62] D Bruneau, F Feuillebois, J Bławdziewicz, and R Anthore. Three-dimensional intrinsic convection in dilute and dense dispersions of settling spheres. *Physics of Fluids*, 10(1):55–59, 1998.
- [63] Wim-Paul Breugem. A second-order accurate immersed boundary method for fully resolved simulations of particle-laden flows. *Journal of Computational Physics*, 231(13):4469–4498, 2012.
- [64] Pedro Costa, Bendiks Jan Boersma, Jerry Westerweel, and Wim-Paul Breugem. Collision model for fully resolved simulations of flows laden with finite-size particles. *Physical Review E*, 92(5):053012, 2015.
- [65] Elisabeth Guazzelli. Evolution of particle-velocity correlations in sedimentation. *Physics of Fluids*, 13(6):1537–1540, 2001.
- [66] Willian Hogendoorn, Wim-Paul Breugem, David Frank, Martin Bruschewski, Sven Grundmann, and Christian Poelma. From nearly homogeneous to core-peaking suspensions: Insight in suspension pipe flows using mri and dns. *Physical Review Fluids*, 8(12):124302, 2023.
- [67] Tariq Shajahan, Thijs Schouten, Shravan KR Raaghav, Cees van Rhee, Geert Keetels, and Wim-Paul Breugem. Characteristics of slurry transport regimes: Insights from experiments and interface-resolved direct numerical simulations. *International Journal of Multiphase Flow*, 176:104831, 2024.
- [68] Wim-Paul Breugem, Vincent Van Dijk, and René Delfos. Flows through real porous media: x-ray computed tomography, experiments, and numerical simulations. *Journal of Fluids Engineering*, 136(4), 2014.
- [69] Wouter Peerbooms, Tim Nadorp, Antoine van der Heijden, and Wim-Paul Breugem. Interparticle friction in sheared dense suspensions: Comparison of the viscous and frictional rheology descriptions. *Journal of Rheology*, 68(2):263–283, 2024.
- [70] Wouter Peerbooms, Antoine van der Heijden, and Wim-Paul Breugem. Transient behavior and steady-state rheology of dense frictional suspensions in pressure-driven channel flow. *Acta Mechanica*, 236(9):5681–5714, 2025.

- [71] Renzo Di Felice. Liquid suspensions of single and binary component solid particles—an overview. *China Particuology*, 5(5):312–320, 2007.
- [72] S Heitkam, Y Yoshitake, F Toquet, D Langevin, and A Salonen. Speeding up of sedimentation under confinement. *Physical review letters*, 110(17):178302, 2013.
- [73] Tariq Shajahan and Wim-Paul Breugem. Influence of concentration on sedimentation of a dense suspension in a viscous fluid. *Flow, Turbulence and Combustion*, 105(2):537–554, 2020.
- [74] Frans TM Nieuwstadt, Jerry Westerweel, and Bendiks J Boersma. *Turbulence: introduction to theory and applications of turbulent flows*. Springer, 2016.
- [75] George J Kynch. A theory of sedimentation. *Transactions of the Faraday society*, 48:166–176, 1952.
- [76] S Leichtberg, Robert Pfeffer, and Sheldon Weinbaum. Stokes flow past finite coaxial clusters of spheres in a circular cylinder. *International Journal of Multiphase Flow*, 3(2):147–169, 1976.

3

Interparticle friction in sheared dense suspensions: Comparison of the viscous and frictional rheology descriptions

In the literature, two different frameworks exist for describing the rheology of solid/liquid suspensions: (1) the 'viscous' framework in terms of the relative suspension viscosity, η_r , as a function of the reduced solid volume fraction, ϕ/ϕ_m , with ϕ_m the maximum flowable packing fraction, and (2) the 'frictional' framework in terms of a macroscopic friction coefficient, μ , as a function of the viscous number, I_v , defined as the ratio of the viscous shear to the wall-normal particle stress. Our goal is to compare the two different frameworks, focusing on the effect of friction between particles. We have conducted a particle-resolved Direct Numerical Simulation study of a dense non-Brownian suspension of neutrally buoyant spheres in slow plane Couette flow. We varied the bulk solid volume fraction from $\phi_b = 0.1$ to 0.6 and considered three different Coulomb friction coefficients: $\mu_c = 0, 0.2$, and 0.39 . We find that η_r scales well with ϕ/ϕ_m , with ϕ_m obtained from fitting the Maron-Pierce correlation. We also find that μ scales well with I_v . Furthermore, we find a monotonic relation between ϕ/ϕ_m and I_v , which depends only weakly on μ_c . Since $\eta_r = \mu/I_v$, we thus find that the two frameworks are largely equivalent and that both account implicitly for Coulomb friction. However, we find that the normal particle stress differences, N_1 and N_2 , when normalized with the total shear stress and plotted against either ϕ/ϕ_m or I_v , remain explicitly dependent on μ_c in a manner that is not yet fully understood.

3.1 Introduction

In many industrial processes, solid-liquid suspensions play an important role, such as in food processing, 3D printing of solid rocket fuels, and solid-liquid fluidized-bed reactors. Next to that, suspensions are commonly encountered in daily life as, for example, in cosmetic products, paints, and fresh concrete. To be able to produce and transport these suspensions in an efficient manner, a thorough understanding of the suspension rheology is required, i.e., the behavior of the suspension under imposed shear.

The rheology of suspensions has been studied extensively for many years since pioneering work by Albert Einstein [3, 4]. A good overview of the subject is given in several review articles [5, 6, 7]. Suspensions show an increase in mixture viscosity, with respect to the viscosity of the carrier fluid, for increasing solid volume fraction. Dense suspensions can exhibit shear rate dependent behavior such as yield stresses [8], shear thinning [9, 10], and (dis)continuous shear thickening [11, 12, 13, 14]. The focus of the present study is on the rheology of monodisperse suspensions of spheres in a Newtonian carrier fluid subject to simple shear. We consider high concentrations but well below the jamming limit. In this case, the suspension viscosity, η , depends on a number of physical parameters, such as the densities of the fluid (ρ_f) and solid phase (ρ_p), the dynamic fluid viscosity (η_0), the sphere diameter (d), the number density of particles per unit volume (n), parameters related to frictional particle contacts (especially the Coulomb coefficient of sliding friction, μ_c), the thermal energy kT (with k the Boltzmann constant and T the temperature), the imposed shear rate ($\dot{\gamma}$), and the time passed since the moment this shear rate was imposed (t) [5],

$$\eta = f(\rho_f, \rho_p, \eta_0, d, n, \mu_c, kT, \dot{\gamma}, t). \quad (3.1)$$

Based on dimensional analysis, these physical parameters can be combined to form the following dimensionless groups:

$$\eta_r = \frac{\eta}{\eta_0}, \quad \phi = n \frac{1}{6} \pi d^3, \quad \rho_r = \frac{\rho_p}{\rho_f}, \quad Pe_{\dot{\gamma}} = \frac{3\pi\eta_0 d^3 \dot{\gamma}}{kT}, \quad Re_{\dot{\gamma}} = \frac{\rho_f d^2 \dot{\gamma}}{\eta_0}, \quad t_r = \frac{t kT}{\eta_0 d^3}, \quad \mu_c, \quad (3.2)$$

where ϕ is the particle volume fraction, $Pe_{\dot{\gamma}}$ is the Péclet number, and $Re_{\dot{\gamma}}$ is the particle Reynolds number based on the applied shear rate. In this work, we will consider neutrally buoyant particles for which $\rho_r = 1$, non-Brownian particles for which $Pe_{\dot{\gamma}} \gg 1$, simple shear in the Stokes regime at $Re_{\dot{\gamma}} = 0.1$, and steady-state conditions $t_r \gg 1$. Given these assumptions, dimensional analysis thus suggests that the relative viscosity depends only on ϕ and μ_c ,

$$\eta_r = f(\phi, \mu_c). \quad (3.3)$$

In his seminal work in the early 1900s, Einstein [3, 4] showed theoretically that for very dilute suspensions up to $\phi \approx 0.05$, when hydrodynamic and contact particle interactions can be ignored, the relative viscosity increases linearly with the particle volume fraction. It was many years later that Batchelor and Green [15] extended his work to moderate concentrations up to $\phi \approx 0.1$ by including hydrodynamic interactions, resulting in a second-order correction term in the expression for the relative viscosity. For simple shear flows the result is given by

$$\eta_r = 1 + \frac{5}{2} \phi + 5.2 \phi^2. \quad (3.4)$$

For concentrations higher than $\phi \approx 0.1$, contact particle-particle interactions cannot be neglected anymore and become increasingly important with increasing concentration. For very high concentrations, the suspension viscosity diverges toward a state in which the suspension stops to flow, known as the jamming transition. The divergence of the viscosity is described by several empirical correlations [16, 17, 18] of which the Maron-Pierce correlation works particularly well for high volume fractions [17],

$$\eta_r = \left(1 - \frac{\phi}{\phi_m}\right)^{-2}. \quad (3.5)$$

Here, ϕ_m is the maximum flowable packing fraction or the volume fraction at which the suspension ceases to flow as the relative viscosity diverges. The maximum flowable packing fraction typically has a value of $\phi_m = O(0.58 - 0.65)$, while the precise value is usually adjusted to provide a best fit with experimental data. Note that the Maron-Pierce correlation does not explicitly depend on μ_c as one would expect based on Equation (3.3) for the dense regime where particle contacts are frequent. However, this dependency is generally assumed to be implicitly contained in ϕ_m , whose value is typically lower for higher values of μ_c [12, 13]. Furthermore, we remark that the Maron-Pierce correlation does not recover Einstein's analytical expression for the dilute regime, and it suggests, though counter-intuitive, that there is still a dependency on ϕ_m in this limit. On the other hand, the Krieger-Dougherty [18] relation for the suspension viscosity

$$\eta_r = \left(1 - \frac{\phi}{\phi_m}\right)^{-2.5\phi_m} \quad (3.6)$$

does recover the Einstein viscosity in the dilute limit but appears less accurate in the very dense regime. Equations (3.5) and (3.6) are equivalent if and only if the maximum flowable packing fraction $\phi_m = 0.8$, although actual values are closer to 0.6.

For spherical particles, which we consider in this work, the relative viscosity has been extensively studied both experimentally [19, 20, 21, 22] and numerically [23, 24, 25, 26, 27, 28, 29] over the years. This has led to a large amount of data for various kinds of particles with different size, roughness, and friction coefficients. The literature has shown that the data collapse fairly well to a master curve when the volume fraction is normalized by the maximum flowable packing fraction ϕ_m , which is dependent on the properties of the particles. The rheology described as a function of the normalized volume fraction ϕ/ϕ_m will be referred to as the *viscous rheology* in the remainder of this work.

In experiments, it is difficult to independently vary the solid friction of the particles; therefore, numerical simulations provide useful insight into the effect of solid friction on the relative viscosity. Sierou and Brady [23] used accelerated Stokesian Dynamics to investigate the flow of hard spheres in shearing flow, reaching volume fractions of up to 60 volume percent. They concluded that the microstructure and rheology are extremely sensitive to particle contacts. Additionally, they observed ordering at volume fractions over $\phi = 0.5$, which affected the relative viscosity. The layering of particles decreased the relative viscosity at these volume fractions with respect to a disordered suspension. Yeo and Maxey [24] performed fully three-dimensional Direct Numerical Simulations (DNS), employing a force-coupling method to study the rheology of suspensions without solid

friction. For the core region of the planar Couette geometry, the relative viscosity showed good agreement with the Eilers correlation [16]; however, for the wall region layering of particles caused disparate results. Gallier et al. [25] studied the effect of the solid friction coefficient on the rheology using DNS, employing a fictitious domain method, finding that the viscosity increases with increasing Coulomb friction coefficient. By separating the hydrodynamic and contact contributions, they showed that the strong increase in relative viscosity near jamming is caused by the contact between particles. More recently, Chèvre-mont et al. [29] used Discrete Element Method (DEM) simulations to study the effect of friction by solving for the particle contact and lubrication forces based on the assumption that the long-range hydrodynamic interactions do not play a role at high volume fractions [27]. They found a similar dependence of the rheology on the friction coefficient and good agreement with previous simulations. Additionally, the experimental data of Boyer et al. [21] showed good agreement with their simulations when a solid friction coefficient of $\mu_c \approx 0.5$ was used.

The relative viscosity is not sufficient to describe the complete rheology of suspensions and is, therefore, not sufficient for constitutive modeling. The microstructure induces anisotropy in the particle stresses under shear, which leads to non-Newtonian behavior [6]. Therefore, the normal stress differences are important for the description of the suspension rheology, which are defined as $N_1 = \Sigma_{11} - \Sigma_{22}$ and $N_2 = \Sigma_{22} - \Sigma_{33}$ for the first and the second normal stress difference, respectively. Here, the subscripts 1, 2, and 3, refer to the direction of the mean flow, velocity gradient, and vorticity, respectively. The normal stress differences are difficult to measure, explaining the sparse experimental literature data and the large discrepancies among different datasets. Experiments [19, 30, 31, 20] and numerical simulations [32, 23, 24, 25, 28] are largely in agreement for the second normal stress difference N_2 , which is negative and increases in magnitude with increasing volume fraction. There is, however, less consensus on the first normal stress difference N_1 . Large variation between datasets and experimental uncertainty give rise to inconclusive results on the sign of N_1 , but for low solid fractions, the magnitude is much smaller than that of N_2 . Some results show a strong increase in magnitude at higher volume fractions, either to positive or negative values. Gallier et al. [26] showed that the large positive values at high volume fraction are caused by wall effects in confined suspensions. Recently, Badia et al. [33] made an effort to develop a continuum model for suspension flow. In that work, they deduced material functions from simulation data in the literature, which include polynomial descriptions of the contact normal stresses and normal stress differences. These polynomials are a function of the normalized volume fraction ϕ/ϕ_m and provide a good fit to a set of data compiled from multiple literature sources [25, 34, 10], suggesting that the normal stresses scale with the normalized volume fraction.

An alternative description of the rheology, not hampered by the divergence of the viscosity near jamming, was introduced by Boyer et al. [21] using insights from the granular flow community. This description, which we will refer to as the *frictional rheology*, describes the suspension rheology in terms of the macroscopic friction coefficient μ and the viscous number I_v . Here, μ is defined as the ratio between the total shear stress and the wall-normal particle stress, $\mu = \sigma_{12}/\sigma_{p,22}$, and I_v is defined as the ratio of the viscous shear stress over the wall-normal particle stress, $I_v = \eta_0 \dot{\gamma}/\sigma_{p,22}$. Using a custom pressure-imposed shear cell on a rheometer, Boyer et al. [21] performed experiments measuring the

contribution of the particles to the wall-normal stress. The shear cell was designed such that the fluid was able to pass through the top plate while keeping this top plate freely moving to impose a normal force to the suspension. Based on the experimental results, Boyer et al. [21] proposed the following relation for the macroscopic friction coefficient:

$$\mu(I_v) = \mu_1 + \frac{\mu_2 - \mu_1}{1 + I_0/I_v} + I_v + \frac{5}{2} \phi_m I_v^{1/2}, \quad (3.7)$$

where $\mu_1 = 0.32$, $\mu_2 = 0.7$, and $I_0 = 0.005$ are empirically determined constants. In Equation (3.7), the first two terms correspond to the contact contribution, whereas the last two terms correspond to the hydrodynamic contribution. Furthermore, they proposed a relation between the solid volume fraction and the viscous number,

$$\phi(I_v) = \frac{\phi_m}{1 + I_v^{1/2}}. \quad (3.8)$$

The frictional rheology is related to the previously discussed viscous rheology through $\eta_r = \mu/I_v$, and from Equations (3.7) and (3.8), Einstein's relation can be recovered in the limit of very large I_v or very small ϕ . Note that this frictional description of the rheology does not explicitly account for interparticle friction. However, both μ and I_v are strongly influenced by interparticle friction in the dense regime, and it is thus assumed to be implicitly accounted for.

Following the introduction of this frictional rheology framework, attempts have been made to improve the model description by adapting the contributions of the hydrodynamic and contact interactions [25, 35, 29]. Gallier et al. [25] took a different approach to obtain the hydrodynamic contribution to the macroscopic friction coefficient, based on the rheological model of Krieger-Dougherty [18], giving

$$\mu^h = I_v + [\eta] \phi_m I_v^{1-n} \quad \text{and} \quad \phi = \frac{\phi_m}{1 + I_v^n}, \quad (3.9)$$

with $[\eta] \approx 2.4$ and $n = 0.4$. Lecampion and Garagash [35] adapted both contributions to the macroscopic friction coefficient without significantly changing the total, leading to

$$\mu(\phi) = \mu_1 + \frac{\phi_m}{\beta} \left(1 - \frac{\phi}{\phi_m} \right) + \left(I_v + \left(\frac{5}{2} \phi_m + 2 \right) I_v^{1/2} \right) \left(1 - \frac{\phi}{\phi_m} \right)^2, \quad (3.10)$$

with $\beta = 0.158$, $\mu_1 = 0.3$, and $\phi_m = 0.585$. Chèvrement et al. [29] proposed changes to the hydrodynamic component of the model by Gallier et al. [25],

$$\mu = \mu_1 + \frac{\mu_2 - \mu_1}{1 + I_0/I_v} + I_v \left(1 - \phi_m \frac{1}{1 + I_v^2} \right)^{-[\eta]}, \quad (3.11)$$

with $\mu_1 = 0.36$, $\mu_2 = 0.7$, $I_0 = 0.0133$, and $[\eta] = 5/2$. Chèvrement et al. [29] found very good agreement with existing data for an I_v range of 5 decades. The literature shows that the frictional rheology is suitable to describe the relation between the shear stress and the wall-normal particle stress for different suspension characteristics and particle properties, with

slightly altered model coefficients. Nevertheless, the frictional rheology framework is, to our knowledge, not thoroughly tested against the normal stresses and stress differences which are needed for a full constitutive set of equations for suspension rheology.

In this chapter, particle-resolved DNS is used to study the rheology of dense non-Brownian suspensions of neutrally buoyant spheres in a Newtonian carrier fluid in plane Couette flow. The Navier-Stokes equations are solved for the fluid phase and the Newton-Euler equations for the solid phase, where the coupling between the phases is numerically accomplished through a computationally efficient Immersed Boundary Method (IBM) [36]. The aim of this study is to compare the viscous to the frictional rheology, i.e., the scaling of the rheology with ϕ/ϕ_m and the viscous number, respectively.

One of the main novelties of our work lies in the advanced numerical method used to investigate the suspension rheology. We use particle-resolved DNS combined with a frictional soft-sphere collision model for particle contacts, which has been extensively validated against experimental data for oblique particle-wall and particle-particle collisions in viscous fluids [37]. Compared to the previous particle-resolved DNS study of Yeo and Maxey [24], our contact model includes tangential friction and stick/slip transition behavior. Gallier et al. [25] used a similar contact model compared to ours in their particle-resolved DNS study, but with a subtle difference in the definition of particle contact related to particle roughness, and their contact force expressions are different from our model except for the Coulomb friction force in the slip regime. Furthermore, we use a larger domain size in our simulations (domain height of 13.5 vs 10 particle diameters) and consider a wider range of bulk solid volume fraction ($\phi_b = 0.1 - 0.6$).

In our study, we consider three different values for the Coulomb coefficient of sliding friction, $\mu_c = 0, 0.2$, and 0.39 , to investigate to what degree ϕ/ϕ_m and I_v account for variations in interparticle friction. The results are used to perform a comprehensive comparison with previous work for the microstructure, stresses, shear rheology, and frictional rheology. To our knowledge, such comprehensive comparison has not been performed since the work of Gallier et al. [25], after which new models were introduced for the frictional rheology [35, 29]. We consider the separate contributions from hydrodynamic and contact interactions to the rheology modeling and investigate in what way the solid friction coefficient affects these contributions. This shows the nuances of modeling the rheology for both the dilute regime, where hydrodynamics dominates, and the dense regime, where the contact interactions are most important. The presentation of our results as a function of both ϕ/ϕ_m and I_v provides insight into the relation between the two rheology descriptions.

3.2 Methods

3.2.1 Governing equations and contact model

The fluid phase is governed by the Navier-Stokes equations that are made dimensionless with the particle diameter as a length scale, $l_{\text{ref}} = d$, the reciprocal of the shear rate as a time scale, $t_{\text{ref}} = 1/\dot{\gamma}$, and the fluid density, ρ_f . These primary scales can be used to derive a velocity scale, $u_{\text{ref}} = \dot{\gamma}d$, and a stress scale, $\sigma_{\text{ref}} = \rho_f d^2 \dot{\gamma}^2$. This leads to the following nondimensional equations:

$$\nabla \cdot \mathbf{u} = 0, \quad (3.12a)$$

$$\left(\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot \mathbf{u}\mathbf{u} \right) = -\nabla p + \frac{1}{Re_{\dot{\gamma}}} \nabla^2 \mathbf{u}, \quad (3.12b)$$

in which $\mathbf{u}$ is the velocity, and p is the pressure. The motions of the spherical particles are governed by the Newton-Euler equations

$$\rho_r \frac{d\mathbf{u}_c}{dt} = \frac{6}{\pi} \left(\oint_{A_p} (\boldsymbol{\sigma}_f \cdot \mathbf{n}) dA + \mathbf{F}_c \right), \quad (3.13a)$$

$$\rho_r \frac{d\mathbf{p}mb\boldsymbol{\omega}_c}{dt} = \frac{60}{\pi} \left(\oint_{A_p} \mathbf{r} \times (\boldsymbol{\sigma}_f \cdot \mathbf{n}) dA + \mathbf{T}_c \right), \quad (3.13b)$$

in which $\mathbf{u}_c$ and $\boldsymbol{\omega}_c$ are the translational and rotational velocity of a particle, respectively; the fluid stress tensor is defined as $\boldsymbol{\sigma}_f = -p\mathbf{I} + \frac{1}{Re_{\dot{\gamma}}} ((\nabla \mathbf{u}) + (\nabla \mathbf{u})^T)$; $\mathbf{n}$ is the outward pointing normal vector; $\mathbf{r}$ is the position vector with respect to the particle centroid; and the final terms, $\mathbf{F}_c$ and $\mathbf{T}_c$, are the force and torque working on the particle as a result of contacts with other particles or the channel walls. The fluid and solid phase are coupled through a no-slip/no-penetration condition on the surface of the particles

$$\mathbf{u} = \mathbf{u}_c + \boldsymbol{\omega}_c \times \mathbf{r} \quad \text{on} \quad A_p. \quad (3.14)$$

Contact between particles is handled using a soft-sphere contact model, including lubrication corrections for short-range particle-particle and particle-wall interactions, which is described in detail by Costa et al. [37]. This contact model is based on a linear spring-dashpot model in which rigid particles are computationally allowed to slightly overlap. The normal contact force is determined using [37]

$$\mathbf{F}_{ij,n} = -k_n \boldsymbol{\delta}_{ij,n} - \eta_n \mathbf{u}_{ij,n}, \quad (3.15)$$

where $\boldsymbol{\delta}_{ij,n}$ is the overlap distance between two particles, $\mathbf{u}_{ij,n}$ is the relative normal velocity of the particles, k_n is the normal spring coefficient, and η_n is the normal damping coefficient. The effect of solid friction is incorporated in the tangential contact force, which accounts for stick/slip transition according to [37]

$$\mathbf{F}_{ij,t} = \min \left(\| -k_t \boldsymbol{\delta}_{ij,t} - \eta_t \mathbf{u}_{ij,t} \|, \| -\mu_c \mathbf{F}_{ij,n} \| \right) \mathbf{t}_{ij}. \quad (3.16)$$

Here, $\boldsymbol{\delta}_{ij,t}$ is the tangential displacement, $\mathbf{u}_{ij,t}$ is the relative tangential velocity, k_t the tangential spring coefficient, η_t the tangential damping coefficient, μ_c the Coulomb coefficient of sliding friction, and $\mathbf{t}_{ij}$ is the surface tangent unit vector.

The contact model coefficients k_n , k_t , η_n , and η_t , depend on the dry normal (e_n) and tangential (e_t) coefficients of restitution and the contact time (T_{con}) [37]. In the present DNS study, we have fixed the latter at $e_n = 0.97$, $e_t = 0.1$, and $T_{con} = 4\Delta t$ with Δt the computational time step. To improve the temporal resolution at which the lubrication and contact forces are resolved, substepping is employed [37] with the number of substeps within a computational time step set to 40 in the current simulations.

We have extensively validated our contact model against experimental data for oblique particle-wall and particle-particle collisions in viscous fluids in a previous study [37]. Our

model is more advanced compared to the work of Yeo and Maxey [24] as it includes also tangential friction. Gallier et al. [25] used a similar contact model, in the sense that their model does include tangential forces and stick-slip transition behavior. However, there is a subtle difference in the definition of particle contact related to particle roughness, and their contact force expressions are different from our model except for the Coulomb friction force in the slip regime. They define the start of particle contact by the moment when the distance between the centroids of two spheres drops below $d + h_r$, with h_r the particle roughness height, while in our case, we assume particle contact to happen when the distance drops below d . In our model, the effect of particle roughness is included explicitly in the lubrication force corrections and implicitly in the parameters of the collision model, notably the Coulomb friction coefficient.

3.2.2 Numerical method and computational setup

The governing equations for the fluid phase are solved on a fully staggered, Cartesian grid using a finite-volume/central-differencing approach combined with a predictor/corrector and third-order Runge-Kutta 3 (RK3) scheme for integration in time. This method is explained in detail by Breugem [36]. For the present simulations in the Stokes regime, the semi-implicit Crank-Nicolson scheme was implemented for integrating the diffusion term in Equation (3.12b). An efficient IBM is used for the fluid/solid coupling, by means of locally adding forces to the Navier-Stokes equations near the boundary of a particle, to enforce Equation (3.14) by good approximation. In the present simulations, this coupling is semi-implicit based on the approach of Tschisgale et al. [38].

The integration of the Newton-Euler equations for the solid phase is performed using the same RK3 scheme. For particles in close proximity, lubrication force corrections are used to account for subgrid hydrodynamic interactions, for which a contribution is added to the contact force. This lubrication force is capped for interparticle distances smaller than the particle roughness, which is assumed to be $0.001d$. The grid resolution used for the simulations is $d/\Delta x = 16$, meaning there are 16 grid cells for the fluid phase over one particle diameter. This resolution was successfully used in the rheological study by Picano et al. [39] in the weakly-inertial regime.

In this work, we consider neutrally buoyant spherical particles, $\rho_r = 1$, that are monodisperse in size. The main parameters that we vary are the bulk volume fraction, which ranges from $\phi_b = 0.1$ to $\phi_b = 0.6$, and the Coulomb coefficient of sliding friction, which is set to $\mu_c = 0$, $\mu_c = 0.2$, and $\mu_c = 0.39$. The value of $\mu_c = 0.39$ is based on the value measured for polystyrene spheres in recent tilted-flume experiments by Shajahan et al. [40]. This gives a total of 24 cases, as specified in Table 3.1. The same friction coefficient is used for interparticle and particle-wall contacts. The computational domain is a rectangular box with dimensions: $L_x = L_z = 13.5d$ and $L_y = 27d$. A schematic of the computational domain is shown in Figure 3.1. The domain is periodic in the x and y directions, while a no-slip/no-penetration boundary condition is imposed on the walls. The shear Reynolds number is set to $Re_{\dot{\gamma}} = 0.1$ for this study. This value is chosen to be in the Stokes regime while still being high enough to allow particles to move over sufficiently large distances during the course of a simulation such that the flow and spatial particle distribution become independent from the initial condition. The particles are initialized by a random positioning in the domain, while making sure there is no overlap between particles and of particles with

the wall. For concentrations above 30%, this random initialization is not feasible anymore. Therefore, a body centered cubic (BCC) structure, with random perturbations in the particle positions, is used for the higher concentrations. The spacing of the BCC structure is adapted to fit the desired number of particles in the domain. The flow is initialized by imposing a linear velocity (plane Couette) profile in the streamwise direction over the entire domain. The initial translational and angular particle velocities are set to the local fluid velocity and half of the local fluid vorticity at the position of the particle centroid. Parameters for the computational setup, as well as derived quantities, are listed in Table 3.1.

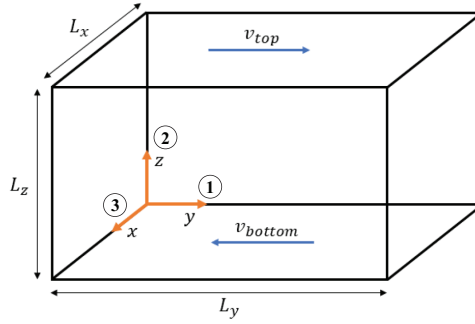


Figure 3.1: Schematic representation of the computational domain indicating the velocities of the top and bottom wall. The numbers along the coordinate axes denote the flow (1), velocity gradient (2), and vorticity (3) directions.

3.2.3 Statistical averaging

The data from the DNS consist of detailed 3-dimensional velocity and concentration fields. These fields need to be averaged over space and time to gain useful insights into the flow dynamics. For plane Couette flow, the mean flow only varies in the wall-normal direction. Therefore, we apply plane-averaging over planes parallel to the walls, followed by averaging over time. For the so-called superficial average of the velocity, this can be expressed as

$$\overline{\langle \mathbf{u}_f \rangle}(z) = \frac{1}{L_x L_y} \sum_x \sum_y \mathbf{u}_f(x, y, z, t) (1 - \alpha(x, y, z, t)) \Delta x \Delta y, \quad (3.17a)$$

$$\overline{\langle \mathbf{u}_p \rangle}(z) = \frac{1}{L_x L_y} \sum_x \sum_y \mathbf{u}_p(x, y, z, t) \alpha(x, y, z, t) \Delta x \Delta y, \quad (3.17b)$$

for the fluid and solid phase, respectively. The brackets and bar denote the spatial averaging and ensemble averaging of samples collected over time, respectively. Here, α is the solid phase indicator function (0 in the fluid and 1 in the particle phase), which is also used to determine the mean local concentration as a function of the wall-normal coordinate using

$$\bar{\phi}(z) = \frac{1}{L_x L_y} \sum_x \sum_y \alpha(x, y, z, t) \Delta x \Delta y. \quad (3.18)$$

Table 3.1: Parameters of the simulated cases: μ_c is the Coulomb coefficient of sliding friction, ϕ_b is the bulk solid volume fraction, N_p is the number of particles, $t_t \dot{\gamma}$ is the transient time of the simulation until the flow is fully developed, $t_s \dot{\gamma}$ is the duration of the simulated steady-state, L_{core} is the width of the core region, L_{wall} is the width of the wall region, ϕ_c is the average solid volume fraction in the core region, and $\dot{\gamma}_c$ is the average shear rate in the core region.

μ_c	ϕ_b	N_p	$t_t \dot{\gamma}$	$t_s \dot{\gamma}$	L_{core}/d	L_{wall}/d	ϕ_c	$\dot{\gamma}_c/\dot{\gamma}$
0	0.1	940	94	102	2.5	5.5	0.104	0.980
0	0.2	1880	94	102	2.5	5.5	0.208	0.980
0	0.3	2819	63	53	2.5	5.5	0.309	0.969
0	0.4	3759	94	61	2.5	5.5	0.410	0.901
0	0.45	4229	109	105	2.5	5.5	0.454	0.876
0	0.5	4699	125	89	2	5.75	0.486	0.831
0	0.55	5169	156	83	1.6	5.95	0.517	0.974
0	0.6	5639	125	114	1.6	5.95	0.565	0.939
0.2	0.1	940	94	94	2.5	5.5	0.109	0.963
0.2	0.2	1880	94	94	2.5	5.5	0.210	0.971
0.2	0.3	2819	63	61	2.5	5.5	0.312	0.954
0.2	0.4	3759	94	52	2.5	5.5	0.410	0.885
0.2	0.45	4229	109	97	2.5	5.5	0.458	0.817
0.2	0.5	4699	94	120	2	5.75	0.503	0.719
0.2	0.55	5169	125	84	1.6	5.95	0.504	0.834
0.2	0.6	5639	125	55	1.6	5.95	0.561	0.879
0.39	0.1	940	94	102	2.5	5.5	0.105	0.975
0.39	0.2	1880	94	102	2.5	5.5	0.210	0.971
0.39	0.3	2819	55	44	2.5	5.5	0.312	0.948
0.39	0.4	3759	63	55	2.5	5.5	0.414	0.860
0.39	0.45	4229	109	105	2.5	5.5	0.460	0.788
0.39	0.5	4699	94	66	1.8	5.85	0.510	0.644
0.39	0.55	5169	156	83	1.6	5.95	0.523	0.473
0.39	0.6	5639	188	45	1.6	5.95	0.580	0.771

Using the superficial averages and the mean local concentration, the intrinsic (phase-averaged) velocities can be computed as

$$\overline{\langle \mathbf{u}_f \rangle^f} = \frac{\overline{\langle \mathbf{u}_f \rangle}}{1 - \bar{\phi}}, \quad (3.19a)$$

$$\overline{\langle \mathbf{u}_p \rangle^p} = \frac{\overline{\langle \mathbf{u}_p \rangle}}{\bar{\phi}}. \quad (3.19b)$$

In addition to the averaging, the superficial (macroscopic) particle stresses need to be computed to describe the rheology of the suspensions. The microscopic particle stress distribution within the particles is not explicitly solved in the DNS as this is not required for rigid particles. However, it can be approximated from the average microscopic stress within a particle, based on the stress distribution on the particle's surface and the contact

forces acting on the particle according to

$$\sigma_{p,ij} \approx \frac{6}{\pi} \left(\oint_{A_p} r_j \sigma_{f,il} n_l dA + \sum r_j F_{c,i} \right), \quad (3.20)$$

where the surface integral is equal to the hydrodynamic particle stresslet for freely rotating particles with zero net torque and the summation accounts for the contribution from the particle contacts. Similar to the superficial velocity averages, the superficial particle stress can be determined as a function of the wall-normal coordinate using

$$\overline{\langle \sigma_{p,ij} \rangle}(z) = \frac{1}{L_x L_y} \sum_{x,y} \sigma_{p,ij}(x, y, z, t) \alpha(x, y, z, t) \Delta x \Delta y. \quad (3.21)$$

Note that $\sigma_{p,ij}$ at the right-hand side of Equation (3.21) is approximated by the *average* stress within a particle and may, therefore, deviate from the *actual* local stress within a particle when the particle stress distribution is strongly *heterogeneous*. As a result, the particle stress profiles may show artificial fluctuations near the wall where the gradients in the solid volume concentration are large due to particle layering. Nonetheless, in the present study, we focus on the rheology in the *homogeneous* core region of the channel for which Equation (3.20) is a good approximation.

3.3 Results

The best way to get a first insight into the suspension behavior is to look at the particle positions and velocities in the domain. A snapshot of the simulations with $\phi_b = 0.5$ is shown in Figure 3.2 for a time instance at which the flow is fully developed. The figure shows the spatial particle distribution and particle velocities in a 3D-slab and two perpendicular cross-sections of the flow domain, for a friction coefficient of $\mu_c = 0$ (a) and $\mu_c = 0.39$ (b). As is visible from the colors, the particles at the top of the domain move in the positive y -direction with the wall velocity and the particles at the bottom move the opposite way with the same velocity. The particles in the interior show a smooth velocity gradient from the bottom to the top of the domain with a velocity close to zero at the centerline. Figure 3.2a, corresponding to a friction coefficient of $\mu_c = 0$, shows that there is a clear particle layering along the walls that extends into the domain over a distance of approximately 4 particle diameters, after which the layering is less distinct. Furthermore, outside this region of particle layering, the particles align in trains that are oriented approximately from the top left toward the bottom right of the domain. This alignment is along the compressional axis of the flow which is the direction in which the most particle contacts are expected for a random particle distribution under shear. The addition of solid friction, shown in Figure 3.2b, results in less distinct wall-induced layering that extends into the domain over a distance of approximately 2 particle diameters. The alignment of particles along the compressional axis is, therefore, also more clearly visible, as the region of the domain where this occurs is larger in this case.

Figure 3.3 shows a snapshot of the particles in the flow for the case with $\phi_b = 0.6$ and $\mu_c = 0.39$. This case shows a pronounced wall-induced layering that extends throughout the entire domain, where the layers of particles at the wall are very neatly aligned in the

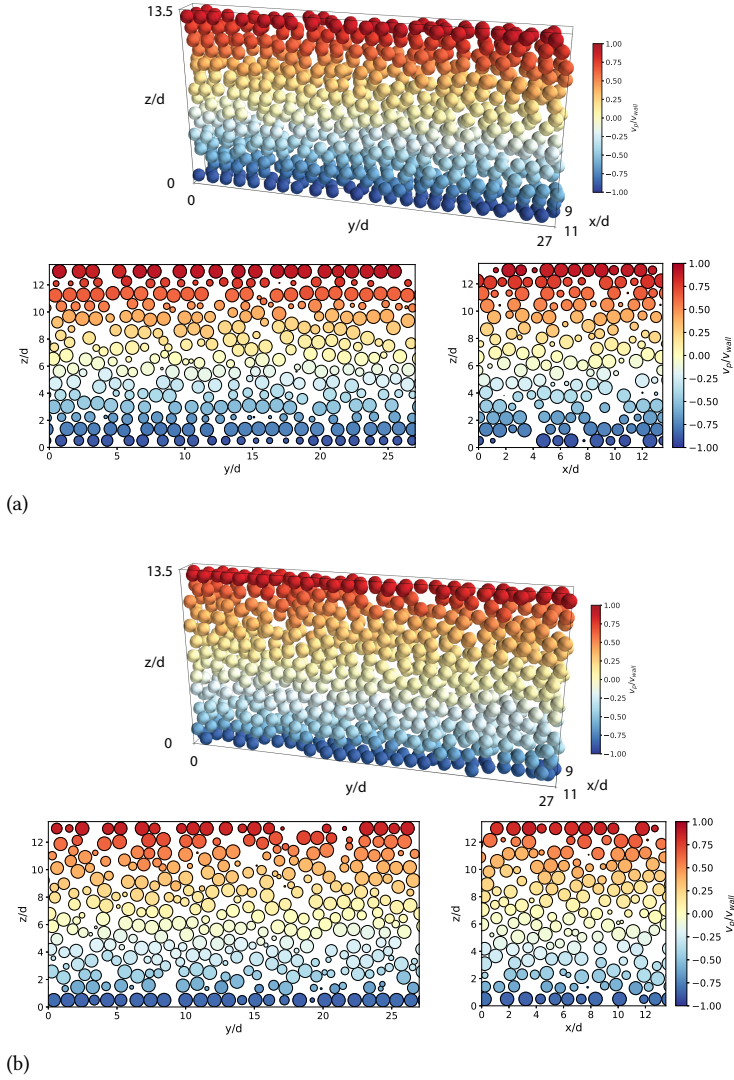


Figure 3.2: Visualization of the particles in a 3D-slab and two perpendicular cross-sections of the flow domain for the cases with $\phi_b = 0.5$ and a friction coefficient of $\mu_c = 0$ (a) and $\mu_c = 0.39$ (b). The particles are colored by their centroid velocity in the flow direction normalized by the wall velocity.

flow direction. Around the centerline of the channel the layers are somewhat distorted but remain clearly visible. The alignment of the particles in the streamwise direction differs strongly from the case with $\phi_b = 0.5$ where the alignment of the particles is along the compressional axis of the flow, indicating a change in dynamics when the solid volume fraction is high enough for the wall-induced ordering to span the entire domain. Moreover, looking at the xz -plane shown in the right pane of Figure 3.3, additional structuring of the

particles is visible. In this plane, the particles are arranged in a hexagonal packing, which is clearly visible in the entire domain.

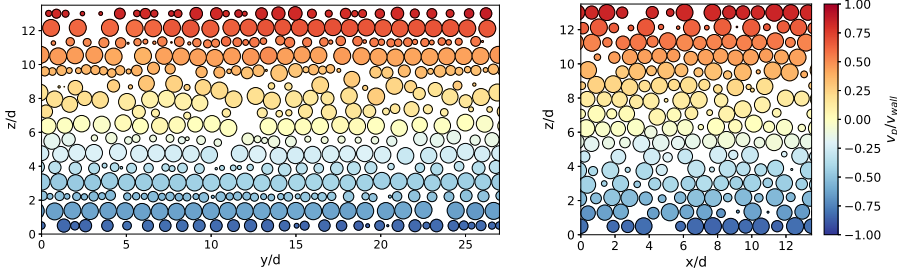


Figure 3.3: Visualization of the particles in two perpendicular cross-sections of the flow domain for the case with $\phi_b = 0.6$ and a friction coefficient of $\mu_c = 0.39$. The particles are colored by their centroid velocity in the flow direction normalized by the wall velocity.

As explained in Section 3.2.3 on statistical averaging, the results of the simulations are plane-averaged in planes parallel to the channels walls. This leads to statistics as a function of the wall-normal coordinate in the channel, which are then time-averaged over the simulated time period in which the flow is fully developed. The resulting concentration profiles are a good way to get an overview of the effect of volume fraction and solid friction on the particle distribution in the suspensions. Figure 3.4 shows the concentration profiles for all cases. These profiles affirm the observation we made in Figure 3.2 that there is particle layering near the wall. The layering is more severe with higher bulk volume fraction and extends into the domain with multiple clear layers for $\phi_b > 0.4$. For the cases with a concentration of $\phi_b \geq 0.55$, the layering even extends throughout the entire domain, as was also observed in Figure 3.3 for the highest concentration. In addition, the concentration profiles show that the wall-induced layering changes from $\phi_b = 0.55$ to $\phi_b = 0.6$, for $\mu_c = 0.39$. This can be seen from the number of peaks in the profiles, equal to 15 and 16 peaks (versus 23 and 24 at the start of the simulation) for $\phi_b = 0.55$ and $\phi_b = 0.6$, respectively. This is in line with the hexagonal packing that was observed in Figure 3.3. The change in layering occurs at a lower volume fraction, between $\phi_b = 0.5$ and $\phi_b = 0.55$, for the suspensions with a lower friction coefficient, showing that the layering is partially mitigated by the increase of solid friction. The increase in friction coefficient also leads to less distinct peaks near the wall, which was previously observed by Gallier et al. [26].

Next to the concentration profiles, we also look at the velocity profiles. The mean intrinsic fluid velocity normalized by the wall velocity is shown in Figure 3.5 for all three friction coefficients. The fluid velocity for the cases without friction shows a slight dependence on the solid volume fraction. For increasing volume fraction, the velocity gradient or shear rate decreases for the region around the center of the channel. This effect is stronger with increasing friction coefficient and clearly visible at $\mu_c = 0.39$. There is a minimum in the shear rate as a function of the bulk volume fraction after which the shear rate increases again. This increase corresponds to the cases with layering throughout the entire domain, showing that this also affects the fluid velocity profile.

In Figure 3.6, we compare the mean intrinsic fluid and particle velocity profiles for the

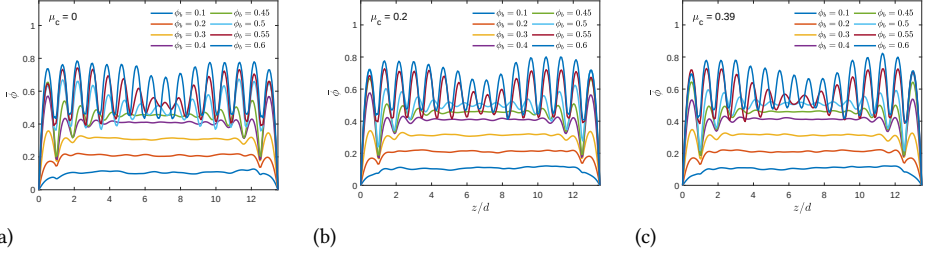


Figure 3.4: Mean solid volume fraction for cases with $\mu_c = 0$ (a), $\mu_c = 0.2$ (b), and $\mu_c = 0.39$ (c) as a function of the wall-normal coordinate.

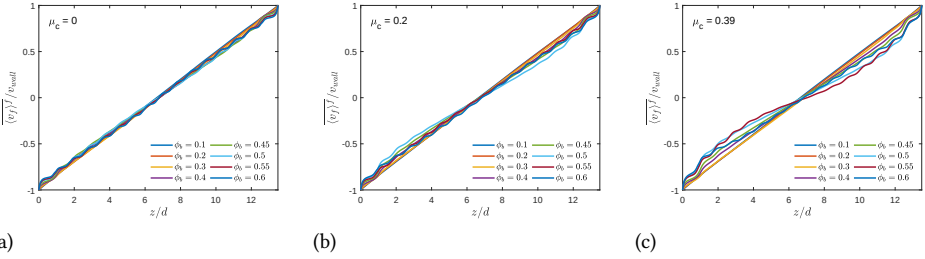


Figure 3.5: Mean intrinsic fluid velocity normalized by the wall velocity for cases with $\mu_c = 0$ (a), $\mu_c = 0.2$ (b), and $\mu_c = 0.39$ (c) as a function of the wall-normal coordinate.

cases with $\phi_b = 0.4$ and for friction coefficients of $\mu_c = 0$ and $\mu_c = 0.39$. While in the core region, the particle and fluid velocity are almost exactly equal, macroscopic particle/fluid slip is observed in the wall region, which is more clearly illustrated in the inset. At the wall ($z/d = 0$) the fluid moves with the velocity of the wall due to the no-slip condition that is enforced there. The particle phase does not have to obey a no-slip condition and shows a slightly lower velocity at the wall. Moving away from the wall the profiles fluctuate somewhat until a position of $z \approx 1.25d$ where the velocity profiles coincide again, showing that the slip only occurs in a thin layer near the wall with a thickness on the order of a particle diameter. Even though the velocity profiles change with friction coefficient, the slip velocity is very similar as well as the width of the layer where the slip occurs for both friction coefficients shown in Figure 3.6.

From the concentration and velocity profiles, we conclude that there is a distinct difference in suspension dynamics between the wall region and the core of the channel. The first notable difference is the wall-induced layering, which originates from the constraint that particles cannot overlap with the flat solid walls and which is amplified by the perfect monodispersity of the spheres. Second, there is significant macroscopic particle-fluid slip in the wall region. This is caused by the no-slip condition for the fluid, while the particles are allowed to slip. The choice of monodisperse spheres and flat walls in the present study was motivated by the simplicity of the system and of the related implementation in our

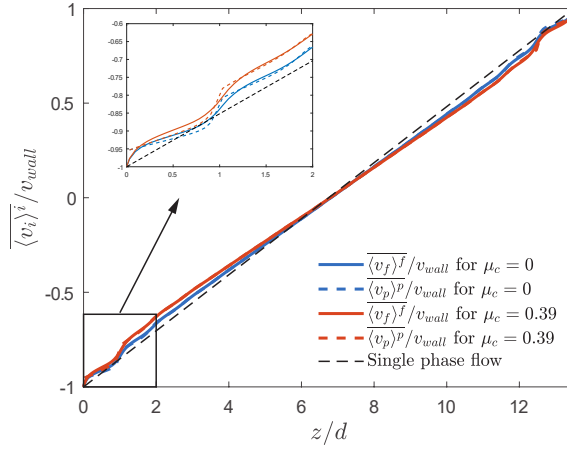


Figure 3.6: Mean intrinsic velocity normalized by the wall velocity for the fluid and solid phase as a function of the wall-normal coordinate, shown for the cases with $\phi_b = 0.4$ and for friction coefficients of $\mu_c = 0$ and $\mu_c = 0.39$. The black dashed line indicates the single phase reference, and the inset shows the slip between phases close to the wall.

in-house particle-resolved DNS code. In the analysis of the suspension rheology, we carefully distinguished between the wall-affected layers on the one hand and the core region with a homogeneous mean concentration and linear mean velocity profile on the other hand. Furthermore, as wall-induced layering becomes progressively more important for increasing bulk concentration, we ignored the cases with the highest bulk concentrations where a homogeneous concentration in the core is absent. In the literature, different methods have been used to counteract the tendency of particle layering along the walls, such as (1) using a bidisperse or polydisperse particle size distribution as these are naturally less prone to ordering [41, 42], (2) exchanging the flat walls for walls with a roughness on the order of the particle size, which is widely used in suspension rheometry [43, 44, 45] and also applied in numerical investigations [46, 47, 48], and (3) using Lees-Edwards (periodic and sliding) boundary conditions [49, 50, 51] for the particles, which removes the constraint that particles cannot overlap with the walls. The use of such methods is recommended for future research, in particular to extend the currently explored range of bulk concentrations in our rheology analysis toward the jamming limit.

The width of the core region, L_{core}/d , is defined around the centerline with a value set to $L_{core}/d = 2.5$ for the cases up to $\phi_b = 0.45$, while set somewhat smaller for the cases with $\phi_b \geq 0.5$, see Table 3.1. We would like to stress the fact that splitting the domain in a wall and a core region makes it possible to obtain an accurate description of the suspension rheology in the statistically homogeneous core with a uniform concentration profile. The cases with $\phi_b \geq 0.55$ for which the wall-layering extends throughout the entire domain are excluded from the analysis and model fits. Figures 3.4 and 3.5 show that the concentration and shear rate in the core region differ slightly from the bulk quantities. For the core, we, therefore, determined the average shear rate ($\dot{\gamma}_c$) and average concentration (ϕ_c), of which the values are also listed in Table 3.1. The cases with $\phi_b = 0.4$ will be used as an

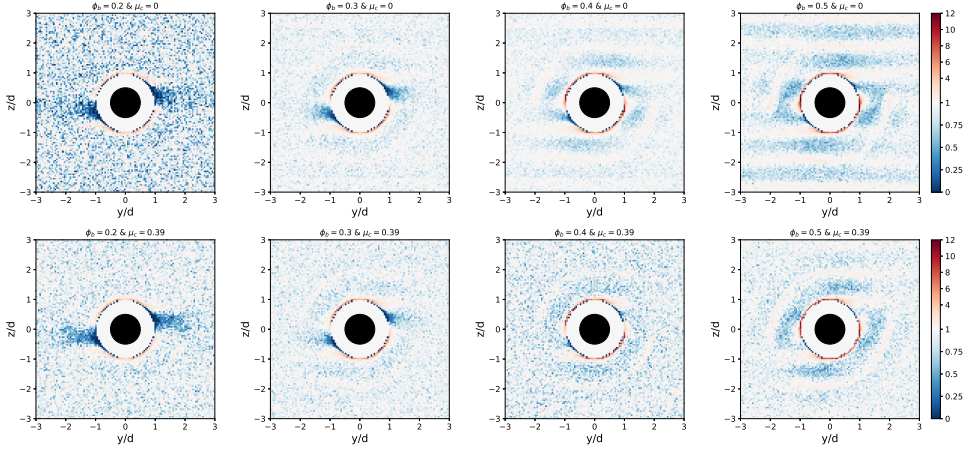
example throughout this work because these cases nicely illustrate the suspension in the dense regime.

In order to investigate the suspension microstructure in the core region, we computed the Particle Pair Distribution Function (PPDF). This expresses the likelihood of finding a neighboring particle at a certain distance and orientation, $\mathbf{r}$, with respect to an arbitrary reference particle in the core region

$$g(\mathbf{r}) = \frac{V/V_{\text{vox}}}{N(N-1)} \sum_p \sum_{p_d} \delta(\mathbf{r} - (\mathbf{x}_{p_d} - \mathbf{x}_p)), \quad (3.22)$$

where V is the total volume of the core region, V_{vox} is the voxel volume of the regular voxel grid used for the calculation, N is the total number of particles in the core region, $\mathbf{x}_p$ is the centroid position of the reference particle, and $\mathbf{x}_{p_d}$ is the centroid position of the neighboring particle. The function δ gives a value of 1 if the particle centroid of the neighboring particle is in the voxel of interest and 0 otherwise. In Equation (3.22), $g(\mathbf{r})$ is normalized such that $g(\mathbf{r}) = 1$ for a statistically homogeneous particle distribution in space. Figure 3.7 shows the PPDFs for a selection of cases with a bulk volume fraction up to $\phi_b = 0.5$ and for friction coefficients of $\mu_c = 0$ and $\mu_c = 0.39$, calculated for the core region of the domain. The color shows the probability of finding another particle centroid at that location, with blue being a lower than average probability and red being higher. Note that the scale of the colorbar is split in two parts at a value of 1, with both red and blue scaling linearly but with different factors. The top row shows the cases with $\mu_c = 0$, while the bottom row shows the cases with $\mu_c = 0.39$. The bulk volume fraction increases from left to right. The PPDFs obtained from our simulations show good qualitative agreement with the experiments of Parsi and Gadala-Maria [52] and Blanc et al. [53], obtained using a Couette rheometer. Our results are also in good agreement with the Stokesian Dynamics simulations of Foss and Brady [54], for their high Péclet cases, and of Sierou and Brady [23]. From the figures, it becomes clear that fewer particles reside near the reference particle in the extensional flow direction, in the so-called depletion zones. The size of these zones becomes smaller with increasing volume fraction and shifts to a position closer to 45° from the positive y -axis. Furthermore, the spots of high probability at $r \approx 1d$ become more prominent with higher volume fraction and shift toward the y -axis, indicating more frequent contact of particles in this direction. This corresponds to the snapshots of the spatial particle distribution and the concentration profiles shown before. For the dense cases, secondary rings of higher than average probability appear at a position of $r \approx 2d$ corresponding to multiparticle interactions. These secondary rings are more clearly visible in the compressional quadrants of the figure, corresponding to the particle trains that we observed in Figure 3.2. Additionally, in the cases without friction horizontal streaks of higher probability are visible for $\phi_b > 0.3$ showing the preference of particles aligning parallel to the wall. It is important to note that this effect is much stronger in the cases without friction, showing that solid friction decreases the tendency for wall-induced layering in dense suspensions.

A convenient way to compare the PPDFs of different cases is to radially average over a thin shell between $1 < r/d < 1.05$ around the particle as a function of the position on the particle. This gives a good indication of the position on the particle where close interactions with neighboring particles occur. Figure 3.8a shows the PPDFs in this thin shell



3

Figure 3.7: PPDF shown for the core region and shear plane. The different panels correspond to different concentrations ($\phi_b = 0.2 - 0.5$, increasing from left to right) and different friction coefficients ($\mu_c = 0$ for top and $\mu_c = 0.39$ for bottom panels). The black disc denotes the reference particle. The shell of $0.5 < r/d < 1$ is blanked out as it is an excluded volume inaccessible to neighboring particles. Note that the scale of the colorbar is linear, but split in two parts, with an eleven times steeper increase for values above 1 than for values below 1.

for the same cases that are shown in Figure 3.7. The angle θ is defined clockwise from the negative y -axis, as depicted in the figure. The first feature that stands out is that the lower theta-bound of the depletion zones ($g < 1$) coincides for all the volume fractions investigated, with and without friction, and is located at approximately $3\pi/4$ and $7\pi/4$, respectively. The width of this depletion zone decreases with increasing volume fraction but seems insensitive to the friction coefficient. Following this depletion zone, a peak develops at $\theta = \pi$ with increasing volume fraction. This peak indicates the alignment of particles parallel to the walls. This alignment is stronger for the cases without friction, which is evident from the larger peak amplitude. The plateaus that are visible for all cases correspond to the compressional quadrants of the shear flow. In this plateau, the probability increases with increasing volume fraction and is mostly insensitive to the friction coefficient. Figure 3.8b shows the PPDF in the shell for the cases with $\phi_b = 0.4$ over a range of $0 < \theta < \pi$. The numerical results of Gallier et al. [25] and Yeo and Maxey [24] are shown for comparison. Our data show very good agreement with the data from the literature.

The applied shear results in stresses inside the microstructure of the suspensions, which can be used to determine the rheology of the suspension. The total shear stress is defined as [cf. Eq. (4.1) in Batchelor [55] and Eq. (7.3) in Guazzelli and Morris [56]]:

$$\overline{\langle \sigma_{12} \rangle} = \frac{1}{Re_{\dot{\gamma}}} \frac{d\overline{\langle v_m \rangle}}{dz} + \overline{\langle \sigma_{p,12} \rangle} - \overline{\langle v_f w_f \rangle} - \rho_r \overline{\langle v_p w_p \rangle}, \quad (3.23)$$

where the first term on the right hand side is the viscous shear stress with $\overline{\langle v_m \rangle} = \overline{\langle v_p \rangle} + \overline{\langle v_f \rangle}$ the mixture velocity, the second term on the right hand side is the particle shear stress, and the last two terms on the right hand side correspond to the Reynolds stresses from fluctuating fluid and particle motions, respectively. The Reynolds stresses are very close to

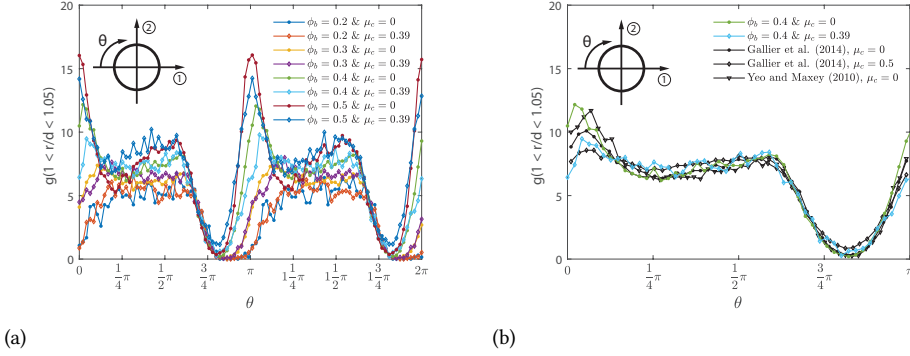


Figure 3.8: PPDFs in the core region, averaged over a thin shell around the reference particle ($1 < r/d < 1.05$) and shown for a selection of cases with bulk volume fractions up to $\phi_b = 0.5$ (a) and comparison of the cases with $\phi_b = 0.4$ with the literature (b).

zero for the present simulations, as expected in the Stokes regime, and are hence omitted in our analysis of the stresses. Figure 3.9 shows the shear stresses for the cases with $\phi_b = 0.4$. Comparing the total stress of the three friction coefficients shows that the shear stress increases with increasing friction coefficient. For all three cases, the total stress is constant in the core region, as expected for a fully developed flow, but fluctuations are observed in the wall regions. The fluctuations are caused by the approximation of the microscopic particle stress within the particles by the particle-averaged value, resulting in a bias when the stress distribution is strongly inhomogeneous as is the case in the wall regions, see the discussion in Section 3.2.3. Irrespective of the friction coefficient, the largest part of the shear stress is the particle stress. This particle stress also accounts for the increase in total stress with increasing friction coefficient, as the viscous stress is similar for all three cases. The particle stress consists of two separate contributions originating from the hydrodynamic interactions $\langle \sigma_{p,12}^{hydro} \rangle$ and the contacts $\langle \sigma_{p,12}^{contact} \rangle$ between particles. These are shown in Figure 3.9 as the dashed and dotted line, respectively. The hydrodynamic contribution is larger than the contact contribution for the cases with $\mu_c = 0$ and $\mu_c = 0.2$, whereas the two contributions are equal for the case with $\mu_c = 0.39$. By increasing the friction coefficient, only the contact contribution to the particle stress increases. This shows that the increase in total shear stress is completely caused by the stress originating from the particle contacts.

Next to the shear stress components, the normal stress components are important for the description of the suspension rheology. Figure 3.10 shows the wall-normal stresses for the cases with $\phi_b = 0.4$. The total wall-normal stress is defined as

$$\langle \sigma_{22} \rangle = -\langle p_f \rangle + \langle \sigma_{p,22} \rangle, \quad (3.24)$$

where the first term is the fluid pressure and the second term is the wall-normal particle stress. We remark that in the DNS a zero reference pressure at the walls is used. Similar to the shear stress, the total stress magnitude increases with increasing friction coefficient.

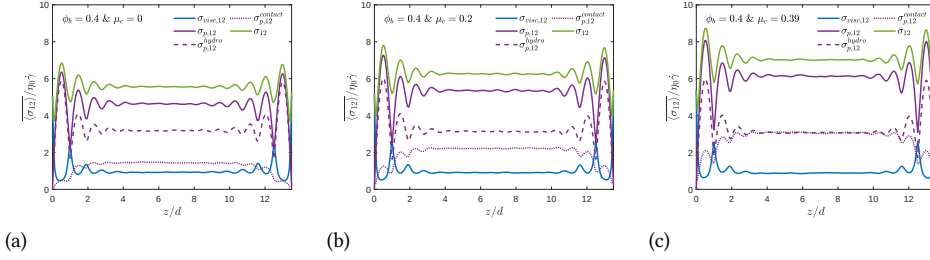


Figure 3.9: Mean shear stresses $\langle \sigma_{i,12} \rangle$ for the cases with $\phi_b = 0.4$ for a Coulomb friction coefficient of $\mu_c = 0$ (a), $\mu_c = 0.2$ (b), and $\mu_c = 0.39$ (c), plotted as a function of the wall-normal coordinate. Dashed lines show the decomposition of the particle stress in a hydrodynamic and contact contribution.

cient. The particle stress provides the largest contribution to the wall-normal stress and moreover is the term that increases with increasing friction coefficient. Decomposing the particle stress into the hydrodynamic contribution $\langle \sigma_{p,22}^{hydro} \rangle$ and the contact contribution $\langle \sigma_{p,22}^{contact} \rangle$, shown as the dashed and dotted line, respectively, shows that the contacts give the largest contribution to the particle stress. Moreover, the hydrodynamic contribution has the opposite sign to the total particle stress and is close to zero.

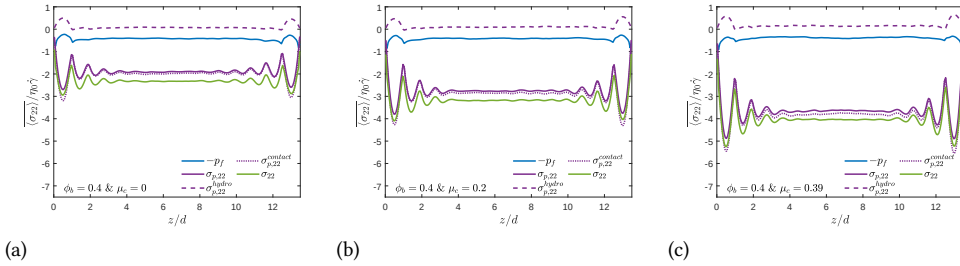


Figure 3.10: Mean wall-normal stresses $\langle \sigma_{i,22} \rangle$ for the cases with $\phi_b = 0.4$ for a Coulomb friction coefficient of $\mu_c = 0$ (a), $\mu_c = 0.2$ (b), and $\mu_c = 0.39$ (c), plotted as a function of the wall-normal coordinate. Dashed lines show the decomposition of the particle stress in a hydrodynamic and a contact contribution.

From the stress budget in the shear plane we can determine the relative viscosity using the total shear stress divided by the viscous shear stress

$$\frac{\eta}{\eta_0} = 1 + \frac{\langle \sigma_{p,12} \rangle}{\frac{1}{Re_\gamma} \frac{\partial \langle v_m \rangle}{\partial z}}. \quad (3.25)$$

Doing this, for all the cases, we can determine the relative viscosity as a function of the volume fraction, which is shown in Figure 3.11a. Our data are shown together with the numerical results of Yeo and Maxey [24] and Gallier et al. [25], as well as the experimental

data from Zarraga et al. [19] and Dbouk et al. [20]. We observe good agreement between our simulations and the results from the literature up to volume fractions of $\phi_b = 0.5$; however, the experimental results show consistently higher relative viscosity over the entire range. The dashed lines show the relative viscosity derived from the frictional rheology model and will be discussed later. The analytical result of Batchelor and Green [15], valid for concentrations up to $\phi \approx 0.1$ and defined in Equation (3.4), is shown for reference as the dashed-dotted line. We observe that our results at $\phi_b = 0.2$ are only slightly higher than predicted from this relation, suggesting a still minor role of contacts at this concentration. From Figure 3.11a we observe that the data does not collapse onto a single curve. A clear influence is present of the friction coefficient, in line with Equation (3.1) based on dimensional analysis. It is only for the lower concentration range, where contacts play a minor role, that the data seem to collapse. For the cases with $\phi_b \geq 0.55$, we observe a deviation from the trend with a decrease in relative viscosity. This deviation can be explained by the layering of particles that we observe for these cases. The particle layering makes it easier for particles to slide past each other, decreasing the resistance to shearing motion and, therefore, decreasing the relative viscosity. The deviation from the trend at high volume fraction is even more visible in Figure 3.11b. This figure shows the relative viscosity as a function of the volume fraction normalized by the maximum flowable packing fraction ϕ_m . The maximum flowable packing fraction is determined by fitting the Maron-Pierce correlation [17], given by Equation (3.5), to the data, excluding the cases with layering throughout the domain. All data collapse to a single curve, showing that the effect of solid friction can be accounted for using the maximum flowable packing fraction. The values of the maximum flowable packing fraction that we find are $\phi_m = 0.70$, $\phi_m = 0.66$, and $\phi_m = 0.64$ for the cases with $\mu_c = 0$, $\mu_c = 0.2$, and $\mu_c = 0.39$, respectively. These values are somewhat higher than those of the experimental datasets from the literature but are in line with the values reported in the numerical studies of Yeo and Maxey [24] and Gallier et al. [25]. It is worthwhile to note that the values for ϕ_m do not change significantly when the cases with $\phi_b = 0.5$ are excluded from the fit, indicating that the core region of these cases is not affected by wall-induced layering.

Figure 3.12 shows the decomposition of the relative viscosity into the hydrodynamic and contact components, where the hydrodynamic part is the sum of the contribution from the viscous stress and the hydrodynamic contribution to the particle stress. The lines show the relative viscosity derived from the frictional rheology model and will be discussed later. In Figure 3.12a it can be seen that for low volume fractions the hydrodynamic component accounts for the largest part of the viscosity. With increasing volume fraction the contact part becomes more important and accounts for the strong diverging nature close to the maximum flowable packing fraction. The effect of friction is not visible in the hydrodynamic part, for which the data overlap in the range of volume fractions considered here. For the contact part, it becomes clear that friction causes a divergence of the relative viscosity at a lower volume fraction. For the frictionless case, it is interesting to note that the hydrodynamic contribution is the largest over the entire range of volume fractions investigated. On the contrary, for the cases with friction the contact contribution exceeds the hydrodynamic contribution for $\phi_c \geq 0.45$. This figure also shows that the breakdown of the diverging trend for the high volume fractions originates primarily from the contact contribution, which decreases for the cases with pronounced layering in

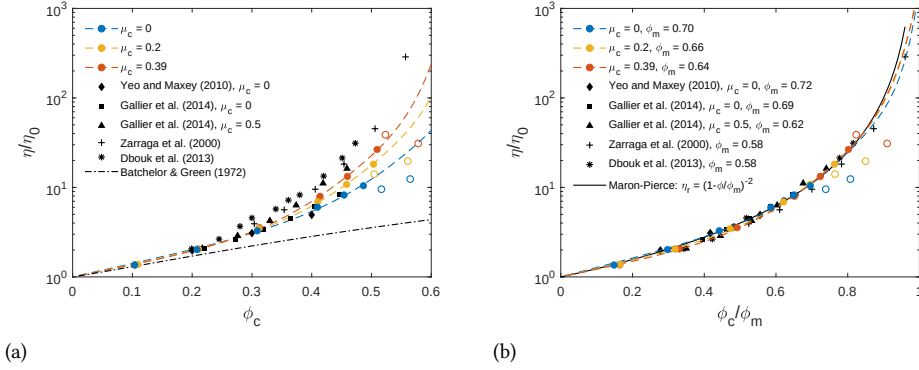


Figure 3.11: Relative viscosity as a function of the volume fraction (a) and the volume fraction normalized by the maximum flowable packing fraction (b), where ϕ_m is determined by fitting the Maron-Pierce correlation [17], Equation (3.5), to the data indicated by the solid line. Colored markers show our data, where the open markers indicate the cases with $\phi_b \geq 0.55$, exhibiting pronounced particle layering, that were excluded from the fit. Black markers show data from the literature [24, 25, 19, 20]. The dashed lines show the relative viscosity derived from the frictional rheology model defined in Equation (3.30) using $\eta_r = \mu/I_v$.

the core region. We again included the analytical expression of Batchelor and Green [15], Equation (3.4), for reference as the dashed-dotted line. The close agreement between our data and this relation at $\phi_b \leq 0.2$ indicates that at low volume fractions the hydrodynamic contribution can be described using this relation. Additionally, this close agreement suggests that the hydrodynamic contribution scales with ϕ_c rather than ϕ_c/ϕ_m . Figure 3.12b shows the decomposition of the relative viscosity as a function of the normalized volume fraction. The normalization causes a collapse of the contact part up to $\phi_c/\phi_m \approx 0.7$, while the effect of the friction coefficient now becomes apparent in the hydrodynamic part of the relative viscosity. This shows that although the relative viscosity collapses with ϕ_c/ϕ_m , the separate contributions do not completely collapse.

As discussed in the Introduction section, an alternative way to describe the shear rheology of suspensions is using the frictional rheology description, where the macroscopic friction coefficient μ is expressed as a function of the viscous number I_v . These can be determined from our simulations using the viscous shear stress over the wall-normal particle stress

$$I_v = \frac{\frac{1}{Re_\gamma} \frac{\partial \langle v_m \rangle}{\partial z}}{-\langle \sigma_{p,22} \rangle}, \quad (3.26)$$

for the viscous number and the total shear stress over the wall-normal particle stress

$$\mu = \frac{\frac{1}{Re_\gamma} \frac{\partial \langle v_m \rangle}{\partial z} + \langle \sigma_{p,12} \rangle}{-\langle \sigma_{p,22} \rangle}, \quad (3.27)$$

for the macroscopic friction coefficient. Figure 3.13a shows the macroscopic friction coefficient as a function of the viscous number. Our data are denoted by the colored markers,

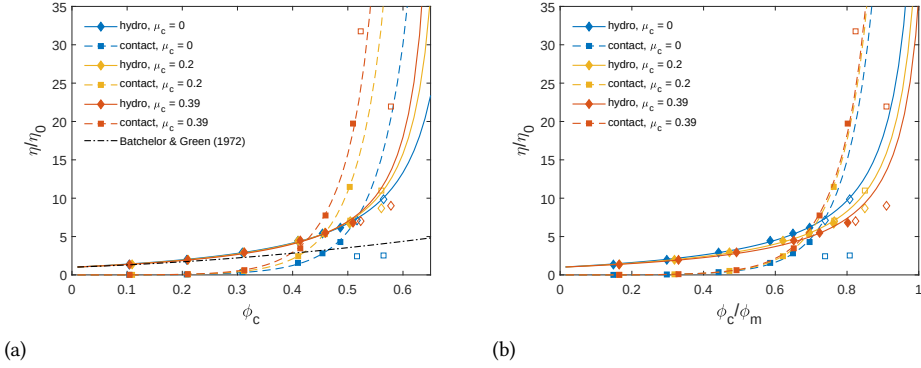


Figure 3.12: Decomposition of the relative viscosity into the hydrodynamic and contact contribution as a function of the volume fraction (a) and the volume fraction normalized by the maximum flowable packing fraction (b). The markers show the DNS results, where the open markers indicate the cases with $\phi_b \geq 0.55$, exhibiting pronounced particle layering. The lines show the relative viscosity derived from the frictional rheology model defined in Equation (3.30) using $\eta_r = \mu/I_v$.

the colored lines present a model description of our data, and the black lines are models from the literature [21, 25, 35, 29]. Comparing our data to the models from the literature shows good agreement at low viscous number (high solid volume fraction); however, at high I_v there is only a qualitative agreement between our data and the models. At these high viscous numbers, our simulations give a consistently higher macroscopic friction than the models predict, for which the model of Gallier et al. [25] is the closest match. The deviation of our data from the models might be caused by the choice for the particle pressure when calculating the viscous number and macroscopic friction coefficient. In the experiments of Boyer et al. [21], a constant particle pressure is imposed; however, it is not entirely clear whether this corresponds to the full normal particle stress or only the contact contribution. Gallier et al. [25] noticed that the agreement between their simulations and the model by Boyer et al. [21] is better when using only the contact contribution to the normal stress. To check the effect on the frictional rheology modeling we tried using the complete wall-normal stress, the wall-normal particle stress, and the contact contribution to the wall-normal particle stress. We decided to use the wall-normal particle stress, based on the results shown in Appendix 3.A. Finally, we note that the deviation seen for high viscous number from the model of Gallier et al. [25] might also be related to subtle differences in the contact modeling; both μ and I_v are normalized with the wall-normal particle stress, which becomes small for high I_v and, hence, is sensitive to how particle contact is dealt with.

A slight deviation from literature models is also present for the relation between the solid volume fraction and the viscous number, as shown in Figure 3.13b. Here, the model of Gallier et al. [25] matches the closest to our data; however, there is still a slight deviation that increases with increasing friction coefficient and is more visible toward the high and low end of the viscous number range. The relations used by Lecampion and Garagash [35], and Chèvrement et al. [29] are identical to the original model proposed by Boyer

et al. [21], defined in Equation (3.8). To model our results, we start with this relation between the viscous number and the solid volume fraction, which we determine by fitting the relation used by Gallier et al. [25] to our data

$$\phi = \frac{\phi_m}{1 + I_v^n}. \quad (3.28)$$

Here, ϕ_m and n are the fitting parameters. To see how well the viscous number collapses the data, we fit Equation (3.28) to each friction coefficient separately. The fits are shown in Figure 3.13b as the colored solid lines, and the fitting coefficients are listed in Table 3.2. The results for all three friction coefficients can be modeled very well separately using this relation, giving values for ϕ_m (see Table 3.2) that are slightly higher than those determined using the Maron-Pierce correlation [17] for the relative viscosity (see legend of Figure 3.11b). However, the similarity in fitting coefficient n indicates that our data might also be modeled using a single value for n .

To model the relation between the macroscopic friction coefficient and the viscous number, the macroscopic friction coefficient is decomposed into its separate contributions. The hydrodynamic part μ^h is shown in Figure 3.13c, together with the corresponding contribution of the literature models. Here, we can see that the model of Gallier et al. [25] shows the best agreement to our data, especially for low I_v . With increasing viscous number, we see that the hydrodynamic contribution is underestimated by all models. Using the model of Gallier et al. [25], as defined in Equation (3.9), we can fit the hydrodynamic contribution to the macroscopic friction coefficient μ^h . Here, ϕ_m and n are already determined, leaving $[\eta]$ as the only fitting coefficient. This fit gives the values of $[\eta]$ for all three solid friction coefficients, which are also listed in Table 3.2. The colored solid lines in Figure 3.13c show that these fits provide a very good description of our data. It is interesting to note that the effect of friction plays a role in the hydrodynamic contribution at low viscous numbers, showing that the hydrodynamic part of the particle shear stress decreases with increasing friction coefficient. At high viscous numbers the fits overlap and show that solid friction does not affect the hydrodynamic contribution in the dilute limit, as expected. The contact part μ^c is shown in Figure 3.13d, which only shows weak dependence on the viscous number over the range investigated in this work. However, the plateau that exists at high viscous number depends on the Coulomb coefficient of sliding friction μ_c . This contradicts the results of Chèvrement et al. [29], who found a plateau value of 0.7 irrespective of the solid friction. They did observe a deviation from the master curve for cases with a low μ_c at lower viscous numbers. There is a limited agreement between our data and the models, which seem to have the right shape but not the right coefficients to describe our data. Our data on the contact contribution show a dependence on the solid friction coefficient, which was also found by Chèvrement et al. [29] but dismissed in their modeling. To be able to fit the contact contribution defined as

$$\mu^c = \mu_1 + \frac{\mu_2 - \mu_1}{1 + I_0/I_v}, \quad (3.29)$$

we need to choose appropriate values for μ_1 as we have no data at very low viscous numbers. To do this, we used the result of Chèvrement et al. [29] by looking at the low I_v plateau in the contact contribution. The values we chose are $\mu_1 = 0.2$, $\mu_1 = 0.3$, and $\mu_1 = 0.36$

for the cases with $\mu_c = 0$, $\mu_c = 0.2$, and $\mu_c = 0.39$, respectively. The resulting fits are shown in Figure 3.13d, and the fitting coefficients μ_2 and I_0 are listed in Table 3.2. The figure shows that Equation (3.29) is able to describe our data very well with fitting coefficients that are of the same order as those found in the literature. Adding the two contributions together provides a description of the complete macroscopic friction coefficient as shown in Figure 3.13a. The colored solid lines are the result of fitting the separate contributions to the contact and hydrodynamic parts, which shows very good agreement to the data. The model, which is essentially the one proposed by Boyer et al. [21] with adjusted coefficients, only shows dependence on the solid friction coefficient in the limit of low viscous numbers. The decomposition of μ shows that the effect of friction is present in both the hydrodynamic and contact contributions, whereas the total does not show this dependence due to compensating effects of friction that cancel each other.

Table 3.2: Fitting coefficients for the frictional rheology model compared to the coefficients found in literature.

	DNS			Boyer et al. [21]	Gallier et al. [25]	Chèvremon et al. [29]
	$\mu_c = 0$	$\mu_c = 0.2$	$\mu_c = 0.39$			
ϕ_m	0.72	0.69	0.67	0.585	0.64	$f(\mu_c)$
n	0.3664	0.3421	0.3309	0.5	0.4	0.5
$[\eta]$	3.53	3.27	3.07	2.5	2.4	2.5
μ_1	0.2	0.3	0.36	0.32	0.32	0.36
μ_2	0.71	0.88	1.04	0.7	0.7	0.7
I_0	0.0194	0.0368	0.0584	0.005	0.005	0.0133

Using Equations (3.9), (3.28), and (3.29), we can derive a relation for the relative viscosity based on the frictional rheology model

$$\eta_r = \frac{\mu^c + \mu^h}{I_v} = \frac{\mu_1}{(\phi_m/\phi - 1)^{1/n}} + \frac{\mu_2 - \mu_1}{(\phi_m/\phi - 1)^{1/n} + I_0} + 1 + [\eta]\phi \left(1 - \frac{\phi}{\phi_m}\right)^{-1}. \quad (3.30)$$

This results in a relative viscosity that is not only a function of ϕ/ϕ_m but also depends on the model coefficients that are, in turn, a function of the solid friction. Equation (3.30) does, however, provide a very good description of the relative viscosity as a function of the solid volume fraction, as can be seen from the dashed lines in Figure 3.11a. At low volume fractions, Equation (3.30) nearly coincides with the Batchelor and Green relation [15], shown by the dashed-dotted line, although in the limit of $\phi \rightarrow 0$ our model does overpredict the Einstein viscosity since $[\eta] > 2.5$. Normalizing the volume fraction by ϕ_m found by the Maron-Pierce fit to the data also shows a collapse for Equation (3.30); however, this does not result in a single curve for different solid friction coefficients, as is shown by the dashed lines in Figure 3.11b, although the difference is small.

The relative viscosity derived from the frictional rheology model can also be decomposed into two separate contributions, with the first two terms in Equation (3.30) accounting for the contacts while the final two terms account for the hydrodynamic contribution. The result of that decomposition is shown as the lines in Figure 3.12. The good agreement between the model and the data show that the frictional rheology and viscous rheology are equivalent with regard to the relative shear viscosity; since $\eta_r = \mu/I_v$ and ϕ/ϕ_m is a

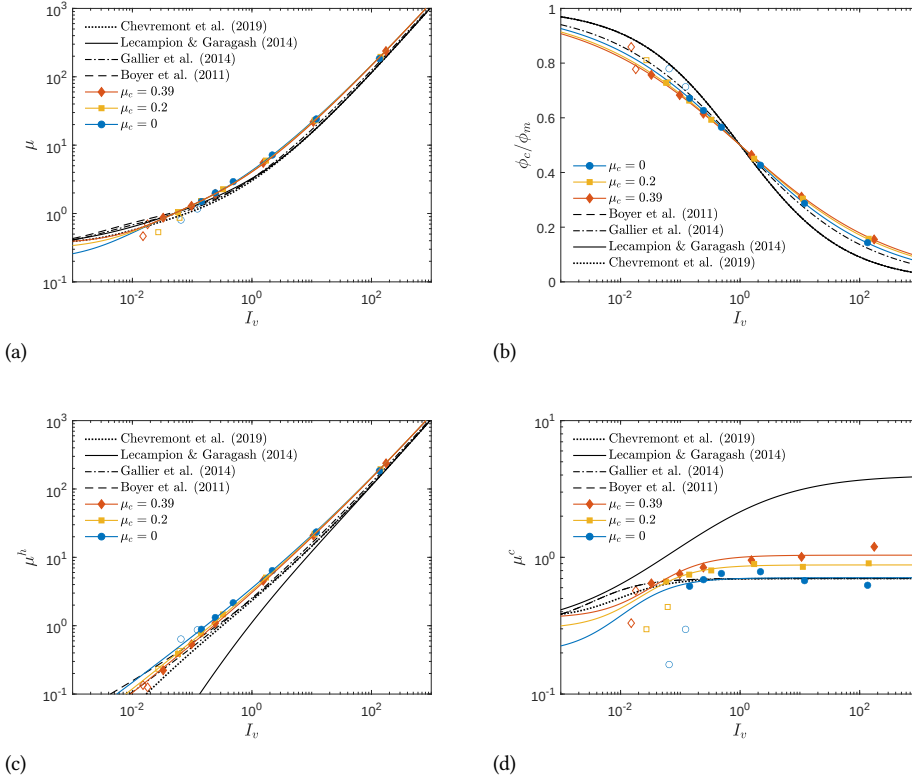


Figure 3.13: Frictional rheology with (a) the macroscopic friction coefficient, (b) the normalized volume fraction, (c) the hydrodynamic part of the macroscopic friction coefficient, and (d) the contact part of the macroscopic friction coefficient as a function of the viscous number. Colored lines show fits to the data, and black lines show models from the literature [21, 25, 35, 29]. Open markers indicate the cases exhibiting pronounced particle layering in the core and were excluded from fits.

monotonically decreasing function in I_v , which is only weakly affected by μ_c , the two frameworks are actually interchangeable. Moreover, the decomposition shows that the hydrodynamic contribution can be described using Equation (3.4) for low volume fractions. Nevertheless, a more detailed investigation on the effect of the Coulomb coefficient of sliding friction on the frictional rheology model is needed. Specifically, investigating how the fitting coefficients change for different Coulomb coefficient of sliding friction.

Having concluded that the frictional rheology and viscous rheology are equivalent with regard to the relative shear viscosity, we turn our attention to the normal stresses. Looking at all three normal stress components, we observe non-Newtonian phenomena that occur in suspensions, which are the anisotropy in the normal stresses and the related anisotropy in the microstructure. Figure 3.14 shows the mean normal particle stresses in the core region of the channel normalized by the mean total shear stress and plotted as a function of the normalized solid volume fraction. The chosen normalizations are

consistent with the viscous rheology framework, noting that the total shear stress scales with the viscous shear stress times a function of ϕ_c/ϕ_m as found above from the shear rheology analysis. Looking at the three different components of the normal stress, $\overline{\langle\sigma_{p,11}\rangle}$, $\overline{\langle\sigma_{p,22}\rangle}$, and $\overline{\langle\sigma_{p,33}\rangle}$ in Figures 3.14a, 3.14b, and 3.14c, respectively, it becomes clear that the normal particle stresses are anisotropic. The effect of friction does not seem to be accounted for in the normalization of the solid volume fraction, ϕ_c/ϕ_m , as the data of the three friction coefficients does not collapse to a single curve, except for the wall-normal particle stress $\overline{\langle\sigma_{p,22}\rangle}$. Plotting the normal stresses as a function of the viscous number would also not result in a collapse of the data with different solid friction coefficients, due to the monotonic relation between ϕ_c/ϕ_m and I_v that is only weakly dependent on μ_c as observed from Figure 3.13b. We remark that the normalization of the normal stresses with the total shear stress is also consistent with the frictional rheology framework, as the total shear stress scales with the wall-normal particle stress times a function of I_v as earlier found from the shear rheology analysis. The effect of layering in the domain is best visible in Figure 3.14a for the streamwise particle stress $\overline{\langle\sigma_{p,11}\rangle}$, where the cases with $\phi_b \geq 0.55$, indicated by the open markers, show a clear deviation from the trend. The lines in the figure represent polynomial fits to the data based on the work of Badia et al. [33] who used these correlations to describe the normal contact stresses in a continuum modeling approach for the suspension rheology. The correlations are defined as

$$\frac{\overline{\langle\sigma_{p,11}\rangle}}{\overline{\langle\sigma_{12}\rangle}} = a_1 \left(\frac{\phi_c}{\phi_m} \right)^{a_2}, \quad (3.31a)$$

$$\frac{\overline{\langle\sigma_{p,22}\rangle}}{\overline{\langle\sigma_{12}\rangle}} = \frac{\overline{\langle\sigma_{p,11}\rangle}}{\overline{\langle\sigma_{12}\rangle}} \left(b_1 + b_2 \frac{\phi_c}{\phi_m} + b_3 \left(\frac{\phi_c}{\phi_m} \right)^2 \right), \quad (3.31b)$$

$$\frac{\overline{\langle\sigma_{p,33}\rangle}}{\overline{\langle\sigma_{12}\rangle}} = \frac{\overline{\langle\sigma_{p,11}\rangle}}{\overline{\langle\sigma_{12}\rangle}} \left(c_1 + c_2 \frac{\phi_c}{\phi_m} + c_3 \left(\frac{\phi_c}{\phi_m} \right)^4 \right). \quad (3.31c)$$

The fitting parameters used to describe our data are shown in Table 3.3 for each of the friction coefficients together with the parameters used by Badia et al. [33] to fit data from the literature. There is some deviation from the coefficients found by Badia et al. [33], which might be caused by the fact that we use the total particle stresses, whereas the original authors used the correlations for the contact part of the stresses. This should only amount to a slight difference as we have seen that, for $\phi_b = 0.4$, the particle stress is almost completely governed by the contact contribution. Figure 3.14d shows the normal stress ratios $\lambda_2 = \overline{\langle\sigma_{p,22}\rangle}/\overline{\langle\sigma_{p,11}\rangle}$ and $\lambda_3 = \overline{\langle\sigma_{p,33}\rangle}/\overline{\langle\sigma_{p,11}\rangle}$ as a function of the normalized volume fraction. This figure shows that the normal stress ratios are similar for all friction coefficients, but do not completely collapse on a single curve. Additionally, λ_2 shows an increase with increasing volume fraction for all three friction coefficients, whereas λ_3 is more or less constant around a value of 0.5 with a slight increase at high volume fractions.

A common way to describe the anisotropy in the normal particle stresses is using the mean normal stress difference

$$N_1 = \overline{\langle\sigma_{p,11}\rangle} - \overline{\langle\sigma_{p,22}\rangle}, \quad (3.32a)$$

Table 3.3: Fitted coefficients of the correlations for the mean normal stresses given by Equations (3.31a) to (3.31c). The columns show the results for $\mu_c = 0$, $\mu_c = 0.2$, and $\mu_c = 0.39$ and reference values from Badia et al. [33].

	$\mu_c = 0$	$\mu_c = 0.2$	$\mu_c = 0.39$	Badia et al. [33]
a_1	-2.3022	-2.3305	-2.3648	-2.4247
a_2	2.7915	2.9724	3.0688	4.1280
b_1	0.9717	0.5938	0.3792	0.3750
b_2	-2.0377	-0.2760	0.4415	0.0366
b_3	2.5687	0.9074	0.3524	0.4846
c_1	0.5895	0.4977	0.3361	2.1446
c_2	-0.5932	-0.3755	-0.0983	-2.7234
c_3	1.8373	1.2661	1.0189	1.5759

$$N_2 = \overline{\langle \sigma_{p,22} \rangle} - \overline{\langle \sigma_{p,33} \rangle}. \quad (3.32b)$$

Figure 3.15 shows the mean normal stress differences, normalized by the mean total shear stress and plotted as a function of the normalized solid volume fraction, together with data and models from the literature. The dashed lines show the mean normal stress differences computed from the fits of Equations (3.31a) to (3.31c) to our data. The first normal stress difference, shown in Figure 3.15a, is slightly negative for volume fractions up to $\phi_c/\phi_m \approx 0.8$ after which there is a strong increase to high positive values. For low volume fractions, our data show good agreement with numerical results from the literature [25, 28] and qualitative agreement to the polynomial description of Badia et al. [33] represented by the solid black line. The shift toward positive values is also present for the literature data and the model; however, the strong increase in our data is caused by the particle layering in the domain at high volume fractions affecting $\overline{\langle \sigma_{p,11} \rangle}$. The first normal stress difference computed from the normal stress fits, shown by the dashed lines, shows good agreement with our data and clearly highlights the effect of friction. With increasing Coulomb friction coefficient, N_1 becomes less negative and the upswing toward positive values is less strong. The second normal stress difference, shown in Figure 3.15b, shows a clear trend toward negative values for high volume fractions. The effect of friction is clearly visible, resulting in a more negative N_2 with increasing friction coefficient, which is stronger at higher volume fractions. This is in good agreement with the data from the literature [25]. Furthermore, the data for the cases with $\mu_c = 0.39$ coincide with the polynomial description of Badia et al. [33], shown by the solid black line, up to the point where the model shows an upswing. The volume fraction at which this happens corresponds to our cases exhibiting a strong layering effect, preventing a good comparison to the model this close to the maximum packing fraction. The second normal stress difference, computed from the normal stress fits and shown by the dashed lines, also shows good agreement with our data. The upswing in the model at high volume fractions is outside the range of our data; however, this upswing is similar to that of the fit of Badia et al. [33] and shifts to lower volume fraction for lower friction coefficient.

The viscous and frictional rheology frameworks fail to collapse the data to a master

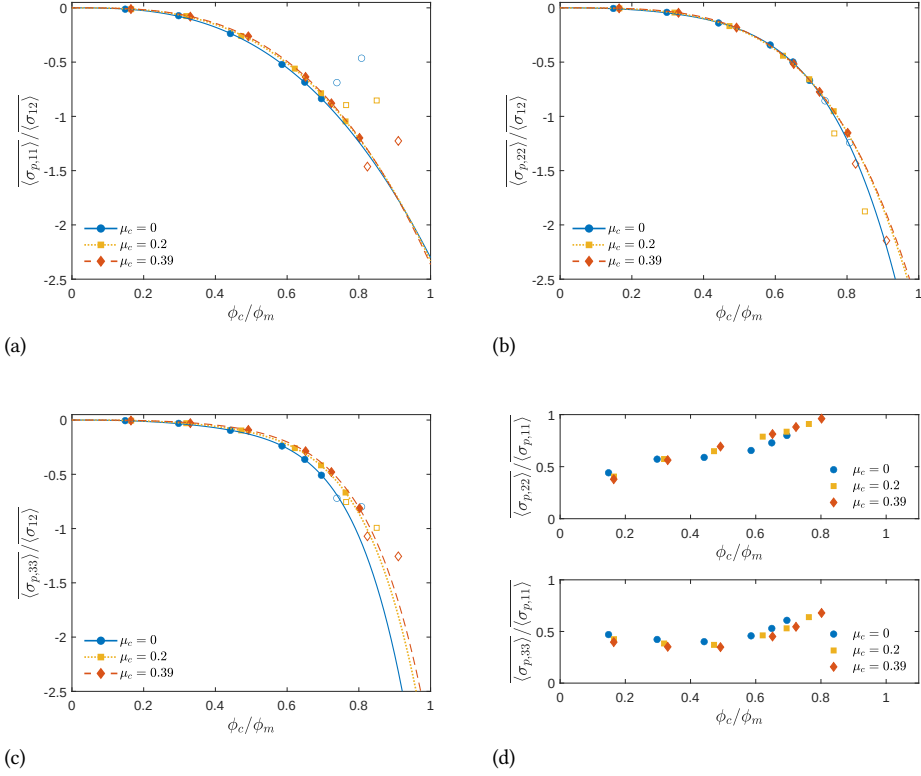


Figure 3.14: Mean normal stresses $\langle \sigma_{p,ii} \rangle$ normalized by the mean total shear stress and plotted as a function of the normalized volume fraction. Lines show fits of Equations (3.31a) to (3.31c) to the data. Open markers indicate the cases with $\phi_b \geq 0.55$, exhibiting strong particle layering in the core and were excluded from the fits.

curve for the normal stresses and, therefore, the normal stress differences, as observed in Figure 3.15 and noting from Figure 3.13b that the monotonic relation between ϕ/ϕ_m and I_v depends only weakly on the friction coefficient. Considering the normalized wall-normal particle stress component $\langle \sigma_{p,22} \rangle / \langle \sigma_{12} \rangle$, we do observe from Figure 3.14 a well-nigh collapse as a function of normalized volume fraction, ϕ_c/ϕ_m , for the three friction coefficients. In passing, we remark that this is consistent with the collapse for μ as a function of I_v in the frictional rheology framework, as $\mu = \langle \sigma_{12} \rangle / \langle \sigma_{p,22} \rangle$ is actually the inverse of the normalized wall-normal particle stress. The other two normal stresses do not collapse as a function of normalized volume fraction, with $\langle \sigma_{p,33} \rangle$ showing the largest effect of the Coulomb friction coefficient. The effect of friction on the normal stress differences we observe matches with data from the literature [25, 28], where there is also no collapse with maximum flowable packing fraction. To complete the description of the suspension rheology, the effect of friction on the normal stress differences needs to be studied in more detail.

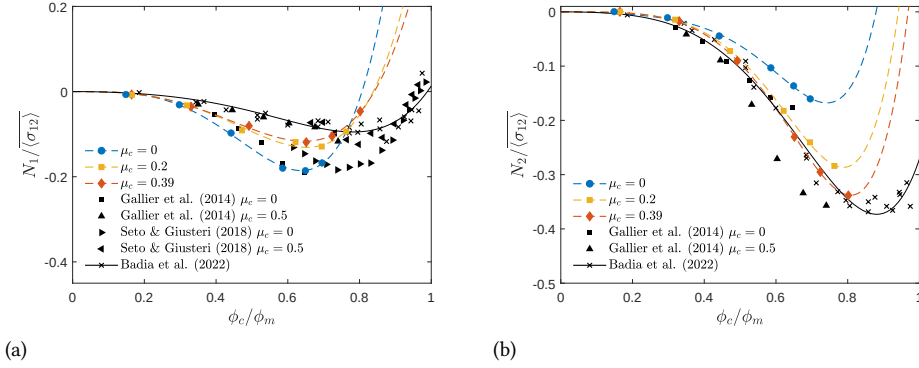


Figure 3.15: Mean normal stress differences N_1 (a) and N_2 (b), both normalized by the mean total shear stress and plotted as a function of the normalized solid volume fraction ϕ_c / ϕ_m . Our data are shown by the colored markers and the dashed lines are the normal stress differences calculated from the fits of Equation (3.31). Black markers indicate data from the literature [25, 28, 33] and the solid line gives a polynomial fit used by Badia et al. [33].

3.4 Conclusions

The particle-resolved simulations of dense suspensions in plane Couette flow performed in this study give a detailed insight into the microstructure and stresses that occur in these suspensions. The effects of solid volume fraction and Coulomb coefficient of sliding friction were shown while comparing the data with experimental and numerical data from the literature. Moreover, we commented on the use of the maximum flowable packing fraction to account for particle characteristics and compared this approach to the frictional rheology framework.

From our results, we can conclude that wall-induced particle layering extends into the entire domain for the cases with volume fractions of $\phi_b \geq 0.55$. This layering affects the rheology by changing the microstructure in a way that particles can slide over each other more easily, lowering the relative viscosity and breaking the diverging trend of the suspension viscosity with increasing concentration. We observed that increasing the solid friction coefficient partially mitigates the layering, which we can see from both the concentration profiles and the PPDFs.

The total shear stress increases with increasing solid volume fraction and increases with increasing friction coefficient. Considering the separate contributions to the total shear stress, we can see that the particle stress accounts for the largest part. This particle stress consists of two parts of which the hydrodynamic part is larger for the low volume fractions, while the contact part dominates for higher volume fractions. The volume fraction at which the contact part becomes larger than the hydrodynamic part decreases with increasing friction coefficient. This can also be seen in the decomposition of the relative viscosity, where the divergence at the lower volume fraction is caused by the increase in the contact particle stress. The relative viscosity, which is in good agreement with the literature, can be collapsed using the maximum flowable packing fraction determined by fitting the Maron-Pierce correlation [17].

The normal stresses show anisotropy leading to nonzero normal stress differences. The normal particle stresses can be described using polynomial fits used by Badia et al. [33] and only show a collapse in ϕ_c/ϕ_m for the wall-normal direction. The normal stress differences show good agreement with the data from the literature, where N_1 is slightly negative for volume fractions up to $\phi_c/\phi_m \approx 0.8$ after which it becomes positive with a large magnitude due to pronounced wall-induced layering. Increasing the friction coefficient decreases the magnitude of N_1 as was also observed in the literature. N_2 is negative over the entire range investigated here and increases in magnitude with volume fraction. The effect of friction is opposite for N_2 , increasing the magnitude with increasing friction coefficient.

Our data can be described using the frictional rheology model from Gallier et al. [25] with adapted fitting coefficients. Additionally, the solid friction coefficient should be taken into account when using the frictional rheology model, and further investigation is needed to incorporate this into the model. The effect of friction is visible when the macroscopic friction coefficient is decomposed into the hydrodynamic and contact parts. These are modeled individually and show that friction slightly lowers the hydrodynamic contribution while it increases the contact contribution. Therefore, the total macroscopic friction coefficient shows the collapse of the data, due to compensating effects of friction on the two individual contributions, with a slight deviation at very low viscous numbers. The relative viscosity derived from the frictional rheology model gives a very good agreement with our DNS data. This indicates that the viscous and frictional rheology frameworks are largely equivalent, primarily because the relative volume fraction ϕ_c/ϕ_m is a monotonic function of I_v and depends only weakly on the friction coefficient. Both frameworks capture the effect of solid friction on the shear rheology. This is, however, not the case for the streamwise and spanwise normal particle stresses as well as the normal particle stress differences, which still show a significant dependency on the friction coefficient that is not yet fully understood.

Appendix

3.A On the normalization with the normal stress in the frictional rheology framework.

The deviation of our DNS results for the frictional rheology from models proposed in the literature might be partially explained by the different choices made in the literature for the normalization with the wall-normal particle stress. In the experiments of Boyer et al. [21], a constant particle pressure is imposed; however, it is not entirely clear whether this corresponds to the full normal particle stress or only the contact contribution. Gallier et al. [25] noticed that the agreement between their simulations and the model by Boyer et al. [21] is better when using only the contact contribution to the normal stress. To check the effect on the frictional rheology modeling we tried using the full wall-normal stress (given by Equation (3.24)), the full wall-normal particle stress, and the contact contribution to the wall-normal particle stress. Figure 3.16a shows the results for the volume fraction in the core region, ϕ_c , as a function of viscous number based on the three different choices for the wall-normal stress. The colors represent the different stress contributions and different symbols are used to distinguish between frictionless and frictional particles. The figure shows that all stress contributions give comparable results. The normalization of the viscous number with the full wall-normal stress, shows the closest match with the model of Boyer et al. [21]; however, toward low viscous number the deviation increases. Using the wall-normal particle stress results in a relatively good agreement with the model of Gallier et al. [25] over the entire range of viscous numbers investigated. The normalization of the viscous number with the contact contribution to the wall-normal particle stress shows the largest deviation from the models at both high and low viscous numbers. At the low viscous number, the deviation might be caused by the pronounced wall-induced layering.

Figure 3.16b shows the macroscopic friction coefficient as a function of the viscous number, where both μ and I_v are defined based on either the full wall-normal stress, the full wall-normal particle stress, or the contact contribution to the wall-normal particle stress. Here, the contributions again give similar results. The particle stress and the contact contribution follow the same curve except at very low I_v . At the high viscous number, the best match with the models is found when using the full wall-normal stress.

Our comparison study shows that the wall-normal stress contribution that is used to determine the frictional rheology has an effect on the results for the frictional rheology, although this effect is limited. Since the flow dynamics in the DNS depends on the pressure gradient instead of pressure itself, and the mean value of the pressure at the walls is arbitrarily set to zero in our simulations for reference, we have chosen not to use the full wall-normal stress but the wall-normal particle stress in the definition of μ and I_v .

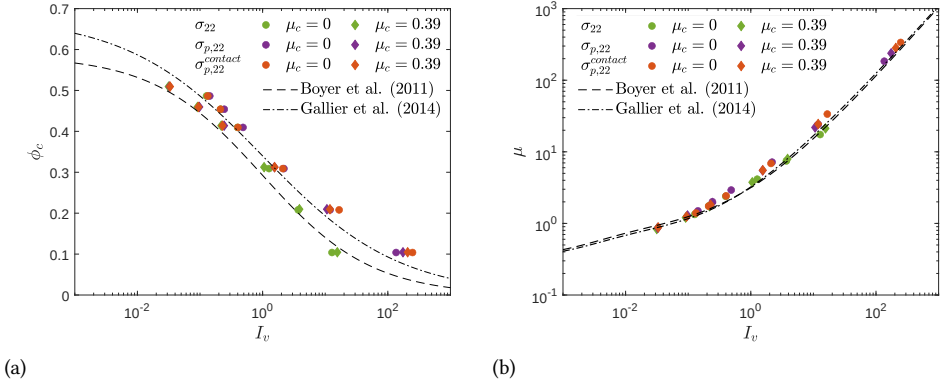


Figure 3.16: Core volume fraction (a) and macroscopic friction coefficient (b) as a function of the viscous number, based on three different choices for the normalization of the wall-normal stress and shown for cases with $\mu_c = 0$ and $\mu_c = 0.39$. The different colors denote normalization with the full wall-normal stress (green), the full wall-normal particle stress (purple) and the contact contribution to the wall-normal particle stress (red). Dots and diamonds denote $\mu_c = 0$ and $\mu_c = 0.39$, respectively. Only data for cases with $\phi_b = 0.1 - 0.5$ is shown, due to the pronounced wall-induced layering observed in the cases with $\phi_b \geq 0.55$.

References

- [1] Wouter Peerbooms, Tim Nadorp, Antoine van der Heijden, and Wim-Paul Breugem. Interparticle friction in sheared dense suspensions: Comparison of the viscous and frictional rheology descriptions. *Journal of Rheology*, 68(2):263–283, 2024.
- [2] Wouter Peerbooms, Tim Nadorp, Antoine E. D. M. van der Heijden, and Wim-Paul Breugem. Data corresponding to the publication: Interparticle friction in sheared dense suspensions: Comparison of the viscous and frictional rheology descriptions. 2024.
- [3] Albert Einstein. *Eine neue Bestimmung der Moleküldimensionen*. PhD thesis, ETH Zurich, 1905.
- [4] Albert Einstein. Berichtigung zu meiner arbeit: Eine neue bestimmung der moleküldimensionen. *Annalen der Physik*, 339(3):591–592, 1911.
- [5] Jonathan J Stickel and Robert L Powell. Fluid mechanics and rheology of dense suspensions. *Annu. Rev. Fluid Mech.*, 37:129–149, 2005.
- [6] Élisabeth Guazzelli and Olivier Pouliquen. Rheology of dense granular suspensions. *Journal of Fluid Mechanics*, 852, 2018.
- [7] Christopher Ness, Ryohei Seto, and Romain Mari. The physics of dense suspensions. *Annual Review of Condensed Matter Physics*, 13:97–117, 2022.
- [8] Abhinendra Singh, Sidhant Pednekar, Jaehun Chun, Morton M Denn, and Jeffrey F Morris. From yielding to shear jamming in a cohesive frictional suspension. *Physical review letters*, 122(9):098004, 2019.
- [9] BM Guy, Michiel Hermes, and Wilson CK Poon. Towards a unified description of the rheology of hard-particle suspensions. *Physical review letters*, 115(8):088304, 2015.
- [10] Laurent Lobry, Elisabeth Lemaire, Frédéric Blanc, Stany Gallier, and François Peters. Shear thinning in non-brownian suspensions explained by variable friction between particles. *Journal of Fluid Mechanics*, 860:682–710, 2019.
- [11] Ryohei Seto, Romain Mari, Jeffrey F Morris, and Morton M Denn. Discontinuous shear thickening of frictional hard-sphere suspensions. *Physical review letters*, 111(21):218301, 2013.
- [12] Romain Mari, Ryohei Seto, Jeffrey F Morris, and Morton M Denn. Shear thickening, frictionless and frictional rheologies in non-brownian suspensions. *Journal of Rheology*, 58(6):1693–1724, 2014.

- [13] Abhinendra Singh, Romain Mari, Morton M Denn, and Jeffrey F Morris. A constitutive model for simple shear of dense frictional suspensions. *Journal of Rheology*, 62(2):457–468, 2018.
- [14] Jeffrey F Morris. Shear thickening of concentrated suspensions: Recent developments and relation to other phenomena. *Annual Review of Fluid Mechanics*, 52:121–144, 2020.
- [15] GK Batchelor and JT Green. The determination of the bulk stress in a suspension of spherical particles to order c^2 . *Journal of Fluid Mechanics*, 56(3):401–427, 1972.
- [16] H Eilers. Die viskosität von emulsionen hochviskoser stoffe als funktion der konzentration. *Kolloid-Zeitschrift*, 97(3):313–321, 1941.
- [17] Samuel H Maron and Percy E Pierce. Application of ree-yring generalized flow theory to suspensions of spherical particles. *Journal of colloid science*, 11(1):80–95, 1956.
- [18] Irvin M Krieger and Thomas J Dougherty. A mechanism for non-newtonian flow in suspensions of rigid spheres. *Transactions of the Society of Rheology*, 3(1):137–152, 1959.
- [19] Isidro E Zarraga, Davide A Hill, and David T Leighton Jr. The characterization of the total stress of concentrated suspensions of noncolloidal spheres in newtonian fluids. *Journal of Rheology*, 44(2):185–220, 2000.
- [20] Talib Dbouk, Laurent Lobry, and Elisabeth Lemaire. Normal stresses in concentrated non-brownian suspensions. *Journal of Fluid Mechanics*, 715:239–272, 2013.
- [21] François Boyer, Élisabeth Guazzelli, and Olivier Pouliquen. Unifying suspension and granular rheology. *Physical review letters*, 107(18):188301, 2011.
- [22] Simon Dagois-Bohy, Sarah Hormozi, Élisabeth Guazzelli, and Olivier Pouliquen. Rheology of dense suspensions of non-colloidal spheres in yield-stress fluids. *Journal of Fluid Mechanics*, 776:R2, 2015.
- [23] Asimina Sierou and John F Brady. Rheology and microstructure in concentrated noncolloidal suspensions. *Journal of Rheology*, 46(5):1031–1056, 2002.
- [24] Kyongmin Yeo and Martin R Maxey. Dynamics of concentrated suspensions of non-colloidal particles in couette flow. *Journal of Fluid Mechanics*, 649:205–231, 2010.
- [25] Stany Gallier, Elisabeth Lemaire, François Peters, and Laurent Lobry. Rheology of sheared suspensions of rough frictional particles. *Journal of Fluid Mechanics*, 757:514–549, 2014.
- [26] Stany Gallier, Elisabeth Lemaire, Laurent Lobry, and Francois Peters. Effect of confinement in wall-bounded non-colloidal suspensions. *Journal of Fluid Mechanics*, 799:100–127, 2016.

- [27] Stany Gallier, François Peters, and Laurent Lobry. Simulations of sheared dense non-colloidal suspensions: Evaluation of the role of long-range hydrodynamics. *Physical Review Fluids*, 3(4):042301, 2018.
- [28] Ryohei Seto and Giulio G Giusteri. Normal stress differences in dense suspensions. *Journal of Fluid Mechanics*, 857:200–215, 2018.
- [29] William Chèvremont, Bruno Chareyre, and Hugues Bodiguel. Quantitative study of the rheology of frictional suspensions: Influence of friction coefficient in a large range of viscous numbers. *Physical Review Fluids*, 4(6):064302, 2019.
- [30] Anugrah Singh and Prabhu R Nott. Experimental measurements of the normal stresses in sheared stokesian suspensions. *Journal of Fluid Mechanics*, 490:293–320, 2003.
- [31] François Boyer, Olivier Pouliquen, and Élisabeth Guazzelli. Dense suspensions in rotating-rod flows: normal stresses and particle migration. *Journal of Fluid Mechanics*, 686:5–25, 2011.
- [32] Anugrah Singh and Prabhu R Nott. Normal stresses and microstructure in bounded sheared suspensions via stokesian dynamics simulations. *Journal of Fluid Mechanics*, 412:279–301, 2000.
- [33] Ayoub Badia, Yves D’Angelo, François Peters, and Laurent Lobry. Frame-invariant modeling for non-brownian suspension flows. *Journal of Non-Newtonian Fluid Mechanics*, 309:104904, 2022.
- [34] François Peters, Giovanni Ghigliotti, Stany Gallier, Frédéric Blanc, Elisabeth Lemaire, and Laurent Lobry. Rheology of non-brownian suspensions of rough frictional particles under shear reversal: A numerical study. *Journal of rheology*, 60(4):715–732, 2016.
- [35] Brice Lecampion and Dmitry I Garagash. Confined flow of suspensions modelled by a frictional rheology. *Journal of Fluid Mechanics*, 759:197–235, 2014.
- [36] Wim-Paul Breugem. A second-order accurate immersed boundary method for fully resolved simulations of particle-laden flows. *Journal of Computational Physics*, 231(13):4469–4498, 2012.
- [37] Pedro Costa, Bendiks Jan Boersma, Jerry Westerweel, and Wim-Paul Breugem. Collision model for fully resolved simulations of flows laden with finite-size particles. *Physical Review E*, 92(5):053012, 2015.
- [38] Silvio Tschisgale, Tobias Kempe, and Jochen Fröhlich. A non-iterative immersed boundary method for spherical particles of arbitrary density ratio. *Journal of Computational Physics*, 339:432–452, 2017.
- [39] Francesco Picano, Wim-Paul Breugem, Dhrubaditya Mitra, and Luca Brandt. Shear thickening in non-brownian suspensions: an excluded volume effect. *Physical review letters*, 111(9):098302, 2013.

- [40] Tariq Shajahan, Thijs Schouten, Shravan KR Raaghav, Cees van Rhee, Geert Keetels, and Wim-Paul Breugem. Characteristics of slurry transport regimes: Insights from experiments and interface-resolved direct numerical simulations. *International Journal of Multiphase Flow*, 176:104831, 2024.
- [41] Sanjeev R Rastogi, Norman J Wagner, and Steven R Lustig. Microstructure and rheology of polydisperse, charged suspensions. *The Journal of chemical physics*, 104(22):9249–9258, 1996.
- [42] Sidhant Pednekar, Jaehun Chun, and Jeffrey F Morris. Bidisperse and polydisperse suspension rheology at large solid fraction. *Journal of Rheology*, 62(2):513–526, 2018.
- [43] Howard A Barnes. A review of the slip (wall depletion) of polymer solutions, emulsions and particle suspensions in viscometers: its cause, character, and cure. *Journal of Non-Newtonian Fluid Mechanics*, 56(3):221–251, 1995.
- [44] Claudia Carotenuto and Mario Minale. On the use of rough geometries in rheometry. *Journal of Non-Newtonian Fluid Mechanics*, 198:39–47, 2013.
- [45] Sebastian Pawelczyk, Marieluise Kniepkamp, Steffen Jesinghausen, and Hans-Joachim Schmid. Absolute rheological measurements of model suspensions: influence and correction of wall slip prevention measures. *Materials*, 13(2):467, 2020.
- [46] Byoungjin Chun, Ilyoung Kwon, Hyun Wook Jung, and Jae Chun Hyun. Lattice boltzmann simulation of shear-induced particle migration in plane couette-poiseuille flow: Local ordering of suspension. *Physics of Fluids*, 29(12), 2017.
- [47] Byoungjin Chun, Jin Seok Park, Hyun Wook Jung, and You-Yeon Won. Shear-induced particle migration and segregation in non-brownian bidisperse suspensions under planar poiseuille flow. *Journal of Rheology*, 63(3):437–453, 2019.
- [48] Nathan J Di Vaira, Łukasz Łaniewski-WoŃk, Raymond L Johnson, Saïed M Aminossadati, and Christopher R Leonardi. Influence of particle polydispersity on bulk migration and size segregation in channel flows. *Journal of Fluid Mechanics*, 939:A30, 2022.
- [49] AW Lees and SF Edwards. The computer study of transport processes under extreme conditions. *Journal of Physics C: Solid State Physics*, 5(15):1921, 1972.
- [50] Eric Lorenz, Alfons G Hoekstra, and Alfonso Caiazzo. Lees-edwards boundary conditions for lattice boltzmann suspension simulations. *Physical Review E*, 79(3):036706, 2009.
- [51] Behnam Khalili and Mahmud Ashrafizaadeh. Implementation of lees–edwards periodic boundary conditions for three-dimensional lattice boltzmann simulation of particle dispersions under shear flow. *Journal of Computational Science*, 68:101982, 2023.
- [52] F Parsi and F Gadala-Maria. Fore-and-aft asymmetry in a concentrated suspension of solid spheres. *Journal of Rheology*, 31(8):725–732, 1987.

- [53] Frédéric Blanc, Elisabeth Lemaire, Alain Meunier, and François Peters. Microstructure in sheared non-brownian concentrated suspensions. *Journal of rheology*, 57(1):273–292, 2013.
- [54] David R Foss and John F Brady. Structure, diffusion and rheology of brownian suspensions by stokesian dynamics simulation. *Journal of Fluid mechanics*, 407:167–200, 2000.
- [55] GK Batchelor. The stress system in a suspension of force-free particles. *Journal of fluid mechanics*, 41(3):545–570, 1970.
- [56] Elisabeth Guazzelli and Jeffrey F Morris. *A physical introduction to suspension dynamics*, volume 45. Cambridge University Press, 2011.

4

Transient behavior and steady-state rheology of dense frictional suspensions in pressure-driven channel flow

Results from particle-resolved Direct Numerical Simulations are presented for dense suspensions of frictional non-colloidal spheres in viscous pressure-driven channel flow. The bulk solid volume fraction varies between $\phi_b = 0.2$ and 0.6 , and the Coulomb friction coefficient is either $\mu_c = 0$ or 0.5 . The main objectives are to unravel the influence of (1) ϕ_b and μ_c on the flow development time and of (2) heterogeneous shear on the steady-state suspension rheology. Starting from an initially homogeneous distribution, the particles show shear-induced migration toward the core until equilibrium is reached. The flow development time decays exponentially with increasing ϕ_b/Φ_R , where Φ_R is a friction-dependent reference bulk concentration beyond which particle contacts cause a rapid increase in the particle stress. The steady-state rheology is studied by means of the ‘viscous’ and ‘frictional’ rheology frameworks. Excluding the central core and wall regions, the data for the local relative suspension viscosity collapse onto a single curve as function of the normalized local concentration $\bar{\phi}/\phi_m$, where ϕ_m is the friction-dependent maximum flowable packing fraction. The frictional rheology shows ‘subyielding’ at low viscous number I_v in the core region, where the macroscopic friction coefficient μ drops below the minimal value found for homogeneous shear flows. A modified frictional rheology model is presented that captures subyielding. Finally, a model is presented for $\bar{\phi}/\phi_{mp}$ as function of I_v , where ϕ_{mp} is a modified maximum flowable packing fraction. It captures both ‘overcompaction’ in the core beyond ϕ_m at high ϕ_b and maximum core concentrations below ϕ_m at lower ϕ_b .

4.1 Introduction

The rheology of dense suspensions is of interest due to the occurrence of suspensions in many natural and industrial applications. One of these applications is the use of suspensions in additive manufacturing, such as for 3D-printing of concrete, metals, food, and energetic materials. The desired solid volume concentration is typically very high for these applications. The complex suspension rheology makes it difficult to control the print quality, especially when the solid volume fraction approaches the maximum flowable packing fraction, ϕ_m .

In the present study, we consider the rheology of monodisperse suspensions of non-colloidal and rigid spheres in a Newtonian fluid. Molecular forces, such as Van der Waals forces, electrostatic forces, and Brownian forces, are assumed to be negligible. Such suspensions may exhibit a yield stress, an anisotropic particle stress tensor with normal stress differences, and shear-thickening behavior at high volume fractions [3]. These phenomena are strongly dependent on the solid volume fraction, ϕ , relative to the maximum flowable packing fraction [4]. The closer the volume fraction is to the maximum flowable packing fraction, the more dominant particle contacts are with respect to particle-fluid and hydrodynamic particle-particle interactions. Therefore, particle size, shape, and surface properties become more important in the very dense regime. In this chapter, we focus on the influence of solid friction between particles, which is known to have a significant impact on the rheology of dense suspensions [5, 6, 7, 8, 9, 10]. Friction also strongly affects the shear-thickening behavior of suspensions [8, 9]; however, we will not address the shear-rate-dependent rheology in the current work. The relative suspension viscosity, η/η_0 with η_0 the viscosity of the carrier fluid, is affected by the solid friction through the maximum flowable packing fraction, as the suspension viscosity diverges at a lower solid volume fraction with increasing Coulomb friction coefficient, μ_c [8]. This is in line with the lower maximum packing fraction for particles with a higher friction coefficient [11, 12].

Many studies have shown that the relative viscosity as a function of solid volume concentration collapses onto a single curve when the concentration is scaled by the maximum flowable packing fraction [13]. Several models for the relative viscosity have been developed over the years. For dilute suspensions, particle-particle interactions are negligible. The theoretical relation for the relative viscosity by Einstein [14, 15] for dilute suspensions gives a linear dependence on the solid volume fraction:

$$\frac{\eta}{\eta_0} = 1 + \frac{5}{2}\phi. \quad (4.1)$$

For suspensions above a volume fraction of $\phi \approx 0.05$, hydrodynamic particle interactions need to be taken into account. This was analyzed by Batchelor and Green [16], who extended the relation of Einstein with an additional term accounting for hydrodynamic particle pair interactions:

$$\frac{\eta}{\eta_0} = 1 + \frac{5}{2}\phi + \xi\phi^2, \quad (4.2)$$

where $\xi = 5.2$ for simple shear flows and $\xi = 7.6$ for pure straining flow. However, this relation fails to capture the strong increase in relative viscosity for $\phi \gtrsim 0.1$ [13]. For these

higher volume fractions, a theoretical derivation of the relative viscosity becomes increasingly difficult due to the many-body hydrodynamic interactions and contacts.

For the higher volume fractions, quite many empirical correlations exist, such as the relation proposed by Krieger and Dougherty [17]:

$$\frac{\eta}{\eta_0} = \left(1 - \frac{\phi}{\phi_m}\right)^{-2.5\phi_m}, \quad (4.3)$$

where ϕ_m is typically obtained from a best fit with experimental data. This relation recovers the Einstein viscosity for low volume fractions, but appears not accurate in the very dense limit. Eilers' relation [18] is in good agreement with empirical data for a large range of volume fractions:

$$\frac{\eta}{\eta_0} = \left(1 + \frac{5\phi/4}{1 - \phi/\phi_m}\right)^2. \quad (4.4)$$

Furthermore, the Maron-Pierce correlation [19] yields good results, especially for high volume fractions [20]:

$$\frac{\eta}{\eta_0} = \left(1 - \frac{\phi}{\phi_m}\right)^{-2}, \quad (4.5)$$

which is similar to the Krieger-Dougherty relation when $\phi_m = 0.8$, but does not recover Einstein's relation in the dilute regime when $\phi_m \neq 0.8$.

Due to the diverging nature of the relative viscosity at high volume fractions, it is difficult to accurately describe the suspension rheology close to the maximum packing fraction. Therefore, Boyer et al. [20] adopted a frictional rheology description from granular mechanics to describe the dense regime of suspension rheology, introducing the viscous number I_v as the governing parameter. The viscous number is defined as the ratio of the viscous shear stress over the wall-normal particle stress, $I_v = -\eta_0 \dot{\gamma} / \sigma_{p,22}$, with $\dot{\gamma}$ the imposed shear rate and $\sigma_{p,22}$ the normal particle stress in the shear plane. Combining this viscous number with a macroscopic friction coefficient, $\mu = -\sigma_{12} / \sigma_{p,22}$, defined as the ratio of the total shear stress (σ_{12}) over the wall-normal particle stress, results in a description of the rheology that is not hampered by the divergence in the relative viscosity close to the maximum packing fraction. Boyer et al. [20] proposed an empirical relation between the solid volume fraction and the viscous number:

$$\phi(I_v) = \frac{\phi_m}{1 + I_v^n}, \quad (4.6)$$

with $n = 0.5$ based on a best fit to their experimental data. Furthermore, Boyer et al. [20] proposed a model for the macroscopic friction coefficient according to:

$$\mu(I_v) = \mu_1 + \frac{\mu_2 - \mu_1}{1 + I_0/I_v} + I_v + \frac{5}{2} \phi_m I_v^{1/2}, \quad (4.7)$$

with $\mu_1 = 0.32$, $\mu_2 = 0.7$, and $I_0 = 0.005$. In Equation (4.7), the first two terms correspond to the particle contact contribution, μ^c , whereas the last two terms correspond to the hydrodynamic contribution, μ^h .

Based on the rheological model of Krieger-Dougherty [17], Gallier et al. [7] took a different approach to obtain the hydrodynamic contribution to the macroscopic friction coefficient, which for large values of I_v is approximately given by:

$$\mu^h = I_v + [\eta]\phi_m I_v^{1-n}, \quad (4.8)$$

with $[\eta] \approx 2.4$ and $n = 0.4$. The value of $n = 0.4$ is also used by Gallier et al. [7] in the relation between the solid volume fraction and the viscous number given by Equation (4.6).

The ‘viscous’ and ‘frictional’ descriptions of the suspension rheology can be related to each other through $\eta/\eta_0 = \mu/I_v$. By construction, the model of Boyer et al. [20], Eqs. (4.6) and (4.7), recovers the correct Einstein limit for $\phi \rightarrow 0$ ($I_v \rightarrow \infty$) and approaches the Maron-Pierce correlation times the constant μ_1 for $\phi \rightarrow \phi_m$ ($I_v \rightarrow 0$). Interestingly, based on a Taylor expansion it can be shown that their model also recovers the relation of Batchelor and Green, Eq. (4.2), for simple shear flows ($\xi = 5.2$) when $\phi_m = 0.697$. The model of Gallier et al. for the hydrodynamic contribution, Eq. (4.8), does not perfectly recover the Einstein limit for small ϕ as the value for $[\eta]$ is slightly smaller than 2.5, although their model yields a better fit with their data for the higher range of volume fractions considered in their study.

The frictional rheologies of Boyer et al. [20] and Gallier et al. [7] are well defined for simple shear flows, with a uniform shear rate such as encountered in plane Couette flow. However, when pressure-driven channel or tube flow is considered, the shear rate becomes spatially heterogeneous, leading to more complex suspension behavior. Moreover, for an initially homogeneous suspension under shear in the Stokes regime, irreversible multiparticle interactions are responsible for shear-induced particle migration from the high-shear regions at the walls toward the low-shear region around the centerline. This process continues until it is counteracted by particle diffusion in the opposite direction [21]. The shear-induced migration is captured fairly successfully by the Suspension Balance Model (SBM) [22, 23, 24]. From a continuum perspective, the particle migration is driven by wall-normal gradients in the wall-normal particle stress [10]. However, literature seems to be inconclusive about the precise origin of the particle stress. For instance, Jamshidi et al. [25] make distinction between the particle-presence stress from hydrodynamic particle interactions and the particle-contact stress from direct particle contacts, and claim that these stresses originate from averaging the momentum equation for the fluid and the particle phase, respectively. This is conceptually different from Morris and Boulay [23], who consider the entire particle stress, including the contribution from hydrodynamic interactions such as lubrication forces, as the result from averaging of the momentum equation for the solid phase only. Furthermore, the SBM relies on the rheological correlations used for the shear and normal particle stresses. In the ‘classical’ SBM formulation [22], the use of the correlations proposed by Boyer et al. [20] and Morris and Boulay [23] results in an equilibrium concentration distribution with a peak at the centerline equal to the maximum packing fraction, contrary to data from experiments and numerical simulations [10]. As will be discussed later, several remedies have been proposed to overcome shortcomings of the classical SBM formulation [26, 27, 28, 29]. Already in the original manuscript in which the SBM was introduced for the first time, Nott and Brady [22] proposed an alternative constitutive relation for the suspension pressure as function of the square root of the

granular temperature (a measure for particle velocity fluctuations) to accommodate non-local suspension behavior in the mean shear rate. This was shown to prevent jamming at the channel centerline, where the mean shear rate reaches zero while the suspension temperature and thus the suspension pressure remain finite.

Next to the modeling of shear-induced particle migration, pressure-driven suspension flows have been studied experimentally for many years [30, 31, 32, 33, 34, 35, 36]. Hampton et al. [30] used Nuclear Magnetic Resonance (NMR) imaging to study the migration of particles in pressure-driven tube flow at bulk concentrations up to $\phi_b = 0.5$ and for two different particle-to-tube radius ratios. Particle migration toward the core was responsible for blunting of the streamwise velocity profile. The streamwise development lengths of the velocity and concentration profiles were found to rapidly decrease for increasing concentration and radius ratio, with a more rapid development of the velocity profile compared to the concentration profile. Lyon and Leal [31, 32] used Laser-Doppler Velocimetry (LDV) combined with density and refractive-index matching of the particles with the suspending fluid, in order to investigate the particle migration in plane channel flow. They found good agreement between the experimentally observed velocity profiles and the model predictions; however, the concentration profiles showed larger deviations, especially close to the channel walls, although this was partially ascribed to the inaccuracy of LDV in these regions. Gao et al. [34] used confocal laser scanning microscopy to study the anisotropic suspension structure for pressure-driven flow in microchannels. They found that pair distribution functions obtained from the experiments, were largely in agreement with results from Stokesian dynamics simulations. Evidence was also shown of local ordering (crystallization) of a fraction of the monosized spheres in the core of the channel, where the solid volume fraction reached a peak value of $\phi = 0.564$. Using Magnetic Resonance Imaging (MRI), Oh et al. [35] performed velocity and concentration measurements on suspensions in pressure-driven pipe flow for bulk solid volume fractions up to $\phi_b = 0.55$. Evidence was reported of compaction of the central particle plug beyond the value of the maximum flowable packing fraction, $\phi_m \approx 0.58$, at the plug boundary up to a random close packing fraction, $\phi_{rcp} \approx 0.64$, at the plug center. Moreover, a model was presented for the concentration and velocity profiles based on the mixture momentum balances for the axial and radial directions. A frictional rheology model was employed for the particle stresses, where compaction in the pipe core was accounted for [27]. The model predictions agreed well with the measured blunted velocity profiles and showed compaction of the central particle plug beyond the maximum flowable packing limit, but failed to capture the shape and extent of the central particle plug. More recently, Rashedi et al. [36] used Particle Image Velocimetry (PIV) combined with a refractive-index matching technique, to record the axial development of the concentration profile in a channel flow for concentrations ranging from $\phi_b = 0.1$ to 0.5 . Their experiments showed that the maximum volume fraction at the centerline increases with bulk volume fraction and saturates at $\phi \approx 0.6$ for bulk volume fractions beyond $\phi_b = 0.3$. These findings also highlight the discrepancy with the ‘classical’ Suspension Balance Model, which predicts a centerline volume fraction equal to the maximum packing fraction, ϕ_m , irrespective of the value of ϕ_b .

Numerical simulations of suspension flows have become more feasible over recent years related to the ever increasing computing power, allowing to perform particle-resolved numerical studies on shear-induced particle migration. Yeo and Maxey [37] used a force-

coupling method to study the dynamics in plane Poiseuille flow for suspensions of frictionless particles with a bulk concentration in the range of $\phi_b = 0.2 - 0.4$. They observed good agreement of the concentration profiles between their numerical results and the experiments of Hampton et al. [30], Lyon and Leal [31], and Gao et al. [33, 34]. Additionally, they showed reasonable agreement between the relative viscosity as a function of the local volume fraction and the earlier mentioned correlations of Krieger and Dougherty [17] and Eilers [18]. A striking observation was the puzzling presence of a negative (positive) particle shear stress just below (above) the channel centerline, opposite to the sign of the local shear rate, and which originated from a negative (positive) contribution from the hydrodynamic particle stresslet. The extension to polydispersity in particle size was studied by Chun et al. [38], using the Lattice-Boltzmann method to simulate segregation of a bidisperse suspension in plane Poiseuille flow at a bulk concentration of $\phi_b = 0.3$. For all investigated particle size and volume fraction ratios, they found that the larger particles preferentially migrate toward the core compared to the smaller particles. The timescale of particle *segregation* appeared to be 5-8 times longer than the timescale for overall particle *migration*, with the latter comparable to the time scale for particle migration in the corresponding monodisperse systems. Di Vaira et al. [39] studied polydisperse systems using a coupled Lattice-Boltzmann/Discrete-Element method. Interestingly, they observed a clear difference in particle segregation for the low and high bulk concentrations investigated: while the larger particles preferentially accumulated in the channel core for $\phi_b \leq 0.3$, there was an increasing preference for the smaller particles to accumulate in the core for $\phi_b \geq 0.4$. The latter was ascribed to the higher shear-rate fluctuations of the smaller particles, which dominate the particle motions in the dense central plug region where the mean shear rate vanishes.

These experimental and numerical studies did not yet lead to a complete description of the suspension dynamics in pressure-driven flows. However, the effort made by Lecampion and Garagash [27] to apply the frictional rheology proposed by Boyer et al. [20] to pressure-driven channel and pipe flow, introduced a clear phenomenological picture of the suspension behavior. Their idea of suspension compaction in the core region was corroborated by the experimental work of Oh et al. [35]. In order to describe this compaction, Lecampion and Garagash [27] proposed a different form of the macroscopic friction coefficient, extending the relation past the maximum flowable packing fraction to account for a jammed particle plug in the center of the channel or pipe:

$$\mu(\phi) = \mu_1 + \frac{\phi_m}{\beta} \left(1 - \frac{\phi}{\phi_m}\right) + \left(I_v + \left(\frac{5}{2}\phi_m + 2\right)I_v^{1/2}\right) \left(1 - \frac{\phi}{\phi_m}\right)^2, \quad (4.9a)$$

$$I_v(\phi < \phi_m) = \left(\frac{\phi_m}{\phi} - 1\right)^2 \quad \text{and} \quad I_v(\phi \geq \phi_m) = 0, \quad (4.9b)$$

where $\beta = -d\phi/d\mu$ for $\mu \rightarrow \mu_1$ represents the so-called compressibility coefficient and is given a value of 0.158 based on a best fit with experimental data in the dense regime. This model allows μ to decrease below $\mu = \mu_1$ by means of a linear extrapolation of the $\phi(\mu)$ relation for a dense suspension under homogeneous shear toward $\mu = 0$. The maximum possible packing fraction of the particle plug is found from substituting $\mu = 0$ and $I_v = 0$ into Eq. (4.9a): $\phi_{rcp} = \phi_m + \beta\mu_1$. For $\phi_m = 0.585$, $\beta = 0.158$ and $\mu_1 = 0.3$ (based on a

best fit with experimental data), $\phi_{rcp} \approx 0.632$, a value representative for a random close packing of monodisperse spheres. More recently, Chèvremont et al. [40] showed that the separate hydrodynamic and contact contributions to Equation (4.9a) do not provide a good description of the frictional rheology in simple shear flow, although the total macroscopic friction coefficient agreed quite well with their numerical simulations.

Based on their proposed frictional rheology model, Lecampion and Garagash [27] also presented analytical solutions for the equilibrium concentration and velocity profiles in fully developed channel and pipe flows. Furthermore, they numerically studied the axial flow development from an initially homogeneous concentration distribution toward equilibrium. The results of these numerical simulations were compared to an analytical expression for the development length, based on the gap-averaged diffusivity evaluated at the channel entrance,

$$L_{dev} = \frac{2}{3} \frac{I_v(\phi_b) S(\phi_b)}{k(\phi_b)} \frac{H^3}{d^2}, \quad (4.10)$$

with d the particle diameter, H the channel half-width, ϕ_b the bulk solid volume fraction, $S(\phi) = -(\mu/\phi)(d\phi/d\mu)$ the so-called inelastic storage coefficient, and $k(\phi) = 2f(\phi)/9\phi$ the normalized permeability. The function $f(\phi)$ is based on the empirical hindered-settling function proposed by Richardson and Zaki [41] and has the form $f(\phi) = (1 - \phi)^n$ with $n \approx 5.1$ used by Lecampion and Garagash [27] for the Stokes regime. Equation (4.10) showed good agreement with the numerical results over the entire range of solid volume fractions. However, comparison to the experimental pipe flow data of Hampton et al. [30] was less successful for the smaller pipe-to-particle diameter ratio and the lower bulk concentrations, ascribed to a too small particle plug in the pipe core and the related breakdown of the continuum model.

Gillissen and Ness [28] highlighted the two main problems of extending the conventional rheology descriptions for homogeneously sheared flows to flows under heterogeneous shear. For pressure-driven channel flow, flow symmetry and the streamwise momentum balance dictate, respectively, a zero mean shear rate and zero mean total shear stress at the channel centerline. According to the frictional rheology model of Boyer et al. [20] given by Eq. (4.7), this would imply jamming at $I_v = 0$, $\phi = \phi_m$ and $\mu = \mu_1$, while experimental observations show *subyielding* with $\mu < \mu_1$ for $I_v > 0$ as well as possible *overcompaction* with $\phi > \phi_m$ in the channel core. Gillissen and Ness [28] proposed a rheological model that incorporates shear stress fluctuations to accommodate subyielding and overcompaction, which was in qualitative agreement with particle-based simulation results.

From the above discussion of the literature, it is clear that the rheology of dense suspensions under heterogeneous shear is far from being fully understood. In the present study, we present results from particle-resolved Direct Numerical Simulations (DNS) for dense suspensions in viscous pressure-driven channel flow. The DNS code is the same as used in our previous study on the rheology of dense suspensions under homogeneous shear [13]. It is based on an efficient Immersed Boundary Method for the fluid/solid coupling [42] and a frictional soft-sphere collision/contact model for particle contacts [43]. We varied the bulk solid volume fraction between $\phi_b = 0.2$ and 0.6. Furthermore, the Coulomb friction coefficient is either $\mu_c = 0$ or 0.5, corresponding to frictionless and frictional particles, respectively. Our main objectives are to gain insight in the influence of (1) ϕ_b and μ_c on

the flow development time and length, and of (2) heterogeneous shear on the steady-state suspension rheology.

This chapter is organized as follows. In Section 4.2 we present the governing equations for the suspension flow, the contact model, the numerical method and the computational setup, and we explain the statistical averaging of the DNS data. In Section 4.3 the results are presented. In the first part, we discuss the transient flow behavior and related particle migration toward the core, and we analyze the flow development time and length until statistical equilibrium is reached. In the second part, we discuss the steady-state rheology. We present results for the mean concentration and velocity profiles, the suspension microstructure, and the stress balances for the streamwise and wall-normal directions. We then analyze the ‘viscous’ suspension rheology in terms of the local relative shear viscosity, η/η_0 , as a function of the normalized local mean concentration, $\bar{\phi}/\phi_m$. This is followed by a discussion of the ‘frictional’ rheology in terms of the macroscopic friction coefficient, μ_c , as a function of the viscous number, I_v . We compare our results with data and models from literature. We present a modified frictional rheology model that accounts for sub-yielding in the channel core. Furthermore, we introduce a model to relate the local mean concentration to the viscous number through normalization with a *modified* maximum packing fraction, which can capture possible overcompaction in the core region. Finally, in Section 4.4 we summarize our main findings and give recommendations for future research.

4.2 Methods

4.2.1 Governing equations and contact model

The fluid phase is governed by the continuity and Navier-Stokes equations that are made dimensionless with the following reference scales¹: $l_{\text{ref}} = d$, $u_{\text{ref}} = v_b$, $t_{\text{ref}} = l_{\text{ref}}/u_{\text{ref}}$, and $m_{\text{ref}} = \rho_f d^3$, where d is the particle diameter, v_b is the bulk mixture velocity, and ρ_f is the fluid phase density. This leads to the following equations:

$$\nabla \cdot \mathbf{u} = 0, \quad (4.11a)$$

$$\left(\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot \mathbf{u} \mathbf{u} \right) = -\nabla p_e - \nabla p + \frac{1}{Re_b(d/2H)} \nabla^2 \mathbf{u}, \quad (4.11b)$$

in which $\mathbf{u}$ is the velocity, ∇p_e is the pressure gradient used to drive the flow at constant bulk velocity, p is the total pressure minus p_e , and Re_b is the bulk Reynolds number defined as $Re_b = \rho_f v_b 2H/\eta_0$ where $2H = L_z$ is the channel height. The particle Reynolds number is based on the wall shear rate of single-phase channel (Poiseuille) flow, $\dot{\gamma}_w = 3v_b/H$, and the particle diameter, and relates to the bulk Reynolds number in the following way:

$$Re_p = \frac{\rho_f \dot{\gamma}_w d^2}{\eta_0} = \frac{3}{2} Re_b \left(\frac{d}{H} \right)^2. \quad (4.12)$$

¹The inertial scaling of the governing equations in the DNS code was chosen merely for pragmatic reasons as we force a constant bulk velocity in our simulations, hence a normalized bulk velocity equal to one. The obtained DNS data was rescaled afterwards in a viscous manner as appropriate for Stokes flow from a physical standpoint (for example, normalization of stresses by $\eta_0 \dot{\gamma}_w$ instead of $\rho_f v_b^2$).

The particle phase is governed by the Newton-Euler equations:

$$\rho_r \frac{d\mathbf{u}_p}{dt} = \frac{6}{\pi} \left(\oint_{A_p} (\boldsymbol{\sigma}_f \cdot \mathbf{n}) dA + \mathbf{F}_c \right), \quad (4.13a)$$

$$\rho_r \frac{d\boldsymbol{\omega}_p}{dt} = \frac{60}{\pi} \left(\oint_{A_p} \mathbf{r} \times (\boldsymbol{\sigma}_f \cdot \mathbf{n}) dA + \mathbf{T}_c \right), \quad (4.13b)$$

in which ρ_r is the ratio between the fluid and solid density; $\mathbf{u}_p$ and $\boldsymbol{\omega}_p$ are the translational and rotational velocity of a particle, respectively; $\boldsymbol{\sigma}_f = -p\mathbf{I} + \frac{1}{Re_b(d/2H)} (\nabla \mathbf{u} + \nabla \mathbf{u}^T)$ is the fluid stress tensor; $\mathbf{n}$ is the outward pointing normal vector; and $\mathbf{r}$ is the position vector with respect to the particle centroid. $\mathbf{F}_c$ and $\mathbf{T}_c$ are the force and torque acting on the particle as a result of contacts with other particles or the channel wall.

The fluid and solid phase are coupled through a no-slip/no-penetration condition on the surface of the particles:

$$\mathbf{u} = \mathbf{u}_p + \boldsymbol{\omega}_p \times \mathbf{r} \quad \text{on } A_p. \quad (4.14)$$

Contact between particles is handled using a soft-sphere contact model including lubrication corrections for short-range particle-particle and particle-wall interactions, which is described in detail by Costa et al. [43]. This contact model is based on a linear spring-dashpot model in which rigid particles are computationally allowed to slightly overlap. The normal contact force is computed from [43]:

$$\mathbf{F}_{ij,n} = -k_n \boldsymbol{\delta}_{ij,n} - \eta_n \mathbf{u}_{ij,n}, \quad (4.15)$$

where $\boldsymbol{\delta}_{ij,n}$ is the overlap distance vector between two particles, k_n is the normal spring coefficient, η_n is the normal dashpot coefficient, and $\mathbf{u}_{ij,n}$ is the relative velocity vector of the particles in the direction parallel to the line of centers. The effect of solid friction is incorporated in the tangential contact force, including the transition from stick to slip behavior when the tangential-to-normal force ratio exceeds a threshold value [43]:

$$\mathbf{F}_{ij,t} = \min \left(\left\| -k_t \boldsymbol{\delta}_{ij,t} - \eta_t \mathbf{u}_{ij,t} \right\|, \left\| -\mu_c \mathbf{F}_{ij,n} \right\| \right) \mathbf{t}_{ij}. \quad (4.16)$$

Here $\boldsymbol{\delta}_{ij,t}$ is the tangential displacement, $\mathbf{u}_{ij,t}$ is the relative tangential velocity, k_t is the tangential spring coefficient, η_t is the damping coefficient, μ_c is the Coulomb coefficient of sliding friction, and $\mathbf{t}_{ij}$ is the surface tangent unit vector.

4.2.2 Numerical method and computational setup

The governing equations for the fluid phase are solved on a fully staggered, Cartesian grid using a finite-volume/central-differencing approach combined with a predictor/corrector scheme and the third-order three-step Runge-Kutta (RK3) scheme for integration in time. This method is explained in detail by Breugem [42]. For the present simulations in the Stokes regime, the semi-implicit Crank-Nicolson scheme was implemented for integrating the diffusion term in Equation (4.11b). An efficient Immersed Boundary Method is used for the fluid/solid coupling, by means of locally adding forces to the Navier-Stokes equations

near the boundary of a particle, to enforce Equation (4.14) by good approximation. As in our previous rheology study [13], the coupling is semi-implicit based on the approach of Tschisgale et al. [44]. The integration of the Newton-Euler equations for the solid phase is performed using the same RK3 scheme, but with substepping for the integration of the contact force and torque to increase the temporal resolution at which particle interactions are resolved [43, 13]. For particles in close proximity, lubrication force corrections are used to account for sub-grid hydrodynamic interactions. Interference of the external shear flow with the local lubrication flow is ignored in these force corrections, since the time scale of the external shear flow is much larger than the characteristic time scale for the lubrication flow. Furthermore, as in our previous study [13], the diverging nature of the lubrication force corrections is capped for interparticle distances smaller than $10^{-3}d$ to mimic the effect of surface roughness on the lubrication flow.

The spatial resolution used for the simulations is $\Delta x/d = 1/16$. This resolution was successfully used in the rheological study by Picano et al. [45] for the weakly-inertial regime and in our previous work on plane Couette flow in the Stokes regime [13]. The time step used for integration of the Navier-Stokes equations over one full Runge-Kutta integration cycle, was chosen sufficiently small to capture the relevant physical time scales in the suspension flow: $\Delta t \dot{\gamma}_w = 1.56 \cdot 10^{-2}$ and $\Delta t \eta_0 / (\rho_f d^2) = 1.56 \cdot 10^{-3}$. Estimating $\dot{\gamma}_{lub} \sim \dot{\gamma} (d/\Delta x)^{3/2}$ as the typical shear rate of the lubrication flow in between two particles moving at a relative normal velocity $\sim \dot{\gamma} d$ and at one grid cell apart, it follows that $\Delta t \dot{\gamma}_{lub} \sim 1$ in our simulations. Interparticle lubrication is thus resolved in time down to gap widths of $\sim \Delta x$ as desired. To further increase the temporal resolution, substepping has been employed with $\Delta t_{sub} = \Delta t/40$ for the integration of the lubrication force correction (for interparticle distances well below Δx) as well as for the contact force and the contact torque [43, 13].

In this work we consider neutrally buoyant spherical particles that are monodisperse in size. The main parameters that we vary are the bulk volume fraction, which ranges from $\phi_b = 0.2$ to $\phi_b = 0.6$ with increments of 0.1, and the Coulomb coefficient of sliding friction, which is set to $\mu_c = 0$ and $\mu_c = 0.5$ for frictionless and frictional particles, respectively. As specified in Table 4.1, this gives a total of 10 cases. The same friction coefficient is used for particle-particle and particle-wall contacts. The computational domain is a square box with dimensions: $L_x = L_y = L_z = 20d$. A schematic of the computational domain is shown in Figure 4.1. The domain is periodic in the x and y directions, while having a no-slip/no-penetration boundary condition in the z -direction. The flow is forced by an applied pressure gradient in the y -direction that is dynamically adjusted to enforce a constant mixture bulk velocity. For clarity, the directions are numbered using (1) for the flow direction, (2) for the wall-normal or velocity gradient direction, and (3) for the spanwise or vorticity direction as indicated in the figure. The particle Reynolds number is set to $Re_p = 0.1$ ($Re_b = 6.67$) for this study. This value is chosen to be in the Stokes regime while still being high enough for computational efficiency. The particles are initialized by a random positioning in the domain, while making sure there is no overlap between particles and with the wall. For concentrations above $\phi_b = 0.3$, this random initialization is not feasible anymore. Therefore, a body-centered cubic (BCC) structure, with random perturbations in the particle positions, is used for the higher concentrations. The spacing of the BCC structure is adapted to fit the desired number of particles in the domain. The flow is initialized by prescribing a parabolic velocity profile for the fluid and particles correspond-

ing to single-phase plane Poiseuille flow. Additionally, the angular particle velocity is set to half the local fluid vorticity.

The DNS code is written in modern FORTRAN with the MPI extension for parallel computing on multi-core systems with distributed memory. The parallelization consists of a 2D pencil decomposition of the computational domain with a controller-worker technique for handling of the particles. The present simulations were partly run on the Dutch National Supercomputer Cartesius and its successor Snellius and partly on an in-house computer cluster, using 100 and 50 CPU cores per simulation, respectively. In total about ~ 2 million CPU hours were used to run all ten simulations and subsequent postprocessing of the data.

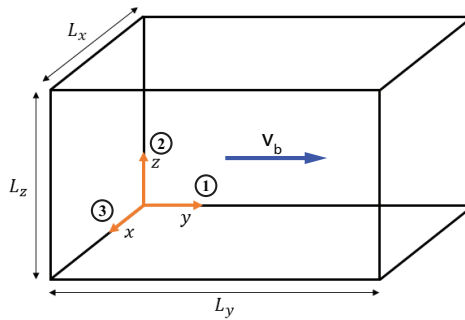


Figure 4.1: Schematic of the computational domain with dimensions: $L_x = L_y = L_z = 20d$. Directions are numbered using (1) for the flow direction, (2) for the wall-normal or velocity gradient direction, and (3) for the spanwise or vorticity direction.

4.2.3 Statistical averaging

The data generated by the numerical method consist of detailed 3-dimensional velocity and concentration fields. These fields are averaged over space and time to gain useful insights into the mean flow dynamics. For fully-developed pressure-driven channel flow, the mean flow and concentration will vary only in the wall-normal direction. Therefore, we apply averaging over thin horizontal slabs with a thickness of 1 grid cell in the wall-normal direction. The so-called superficial averages of the fluid and particle velocities are denoted by brackets and defined by, respectively:

$$\overline{\langle \mathbf{u}_f \rangle}(z) = \frac{1}{L_x L_y \Delta z} \sum_x \sum_y \mathbf{u}_f(x, y, z, t) (1 - \alpha(x, y, z, t)) \Delta x \Delta y \Delta z, \quad (4.17a)$$

$$\overline{\langle \mathbf{u}_p \rangle}(z) = \frac{1}{L_x L_y \Delta z} \sum_x \sum_y \mathbf{u}_p(x, y, z, t) \alpha(x, y, z, t) \Delta x \Delta y \Delta z, \quad (4.17b)$$

where the bar denotes ensemble averaging of samples collected over time. Here α is the solid phase indicator function, which is also used to determine the mean concentration

Table 4.1: Parameters of the simulated cases: μ_c is the Coulomb coefficient of sliding friction, ϕ_b is the bulk solid volume fraction, N_p is the number of particles, $t_{tot} v_b/d$ is the total simulated time, $t_{dev} v_b/d$ is the *estimated* flow development time, “steady state” indicates whether or not fully developed flow was reached, N_{fields} is the number of sample fields in steady state used for statistical averaging, $t_{int} v_b/d$ is the time interval between the consecutive sample fields, $\bar{\phi}_i$ is the mean solid volume fraction in region i (wall, intermediate, or core region), and z_{core}/d is the wall-normal position at which the core region starts (the upper end of the core region is given by $(L_z - z_{core})/d$).

μ_c	0					0.5				
ϕ_b	0.2	0.3	0.4	0.5	0.6	0.2	0.3	0.4	0.5	0.6
N_p	3056	4584	6112	7639	9167	3056	4584	6112	7639	9167
$t_{tot} v_b/d$	3125	5208	5208	2604	2083	3125	5010	3125	2083	1562
$t_{dev} v_b/d$	12490	11554	4243	1885	1164	10382	4599	2276	1054	458
steady state	no	no	yes	yes	yes	no	yes	yes	yes	yes
N_{fields}			180	130	170		80	150	200	200
$t_{int} v_b/d$			5.21	5.21	5.21		5.21	5.21	5.21	5.21
$\bar{\phi}_{wall}$			0.28	0.40	0.55		0.20	0.28	0.38	0.49
$\bar{\phi}_{inter}$			0.39	0.49	0.61		0.30	0.39	0.48	0.61
$\bar{\phi}_{core}$			0.52	0.59	0.62		0.41	0.51	0.58	0.64
z_{core}/d			6.91	6.53	4.78		7.34	6.66	5.41	3.10

profile as a function of the wall-normal coordinate using:

$$\bar{\phi}(z) = \frac{1}{L_x L_y \Delta z} \sum_x \sum_y \alpha(x, y, z, t) \Delta x \Delta y \Delta z. \quad (4.18)$$

Using the superficial averages and the concentration profile, the so-called intrinsic (phase-averaged) averages can be computed:

$$\overline{\langle \mathbf{u}_f \rangle^f} = \frac{\overline{\langle \mathbf{u}_f \rangle}}{1 - \bar{\phi}}, \quad (4.19a)$$

$$\overline{\langle \mathbf{u}_p \rangle^p} = \frac{\overline{\langle \mathbf{u}_p \rangle}}{\bar{\phi}}. \quad (4.19b)$$

In addition to the averaging, the particle stresses need to be computed to describe the rheology of the suspensions. The microscopic particle stress is not explicitly solved in the DNS, but the averaged value within a particle can be computed from the stress distribution on the particle’s surface according to:

$$\sigma_{p,ij} \approx \frac{6}{\pi} \left(\oint_{A_p} r_j \sigma_{f,il} n_l dA + \sum r_j F_{c,i} \right), \quad (4.20)$$

where the surface integral is equal to the hydrodynamic particle stresslet for freely rotating particles with zero net torque and the summation accounts for the contribution from the

particle contacts. Similar to the superficial velocity averages, the superficial particle stress can be determined as a function of the wall-normal coordinate using:

$$\overline{\langle \sigma_{p,ij} \rangle}(z) = \frac{1}{L_x L_y \Delta z} \sum_{x,y} \sigma_{p,ij}(x, y, z, t) \alpha(x, y, z, t) \Delta x \Delta y \Delta z. \quad (4.21)$$

Note that $\sigma_{p,ij}$ at the right-hand side of Equation (4.21) is approximated by the *average* stress within a particle and may therefore deviate from the *actual local* stress within a particle when the particle stress distribution is strongly heterogeneous. As a result, the particle stress profiles show artificial oscillations near the wall where the gradients in the solid volume concentration are large due to particle layering.

4.3 Results and discussion

4

The investigation of the rheology and the effect of solid friction in pressure-driven plane channel flow can be split in two parts: the transient in which particle migration takes place, and the fully-developed flow after the migration is completed. The effect of friction on the particle migration will be discussed first. In this part, we will look at the development of the concentration and velocity profiles as well as the timescale of particle migration. The second part will focus on the description of the rheology of the suspensions in fully-developed flow and the effect of solid friction on the rheology. The rheology is studied in terms of velocity and concentration profiles, particle pair distribution functions, stress balances, relative viscosity, normal stress differences, and the frictional rheology.

4.3.1 Particle migration

The migration of particles in our numerical simulations becomes evident when looking at the spatial particle distribution over time, as shown in Figure 4.2. These figures show the particles in a yz cross-section of the domain at a fixed x -position for the case with $\phi_b = 0.4$ and $\mu_c = 0$. The time instants for these snapshots are given as a fraction of the time, t_{dev} , for the suspension to become fully developed; the precise definition will be given later. In this case $t = 0.2t_{dev}$, $t = 0.6t_{dev}$, and $t = t_{dev}$ are chosen to show the migration of the particles from an initially homogeneous distribution at $t = 0$. At $t = 0.2t_{dev}$, it is already visible that the core of the channel is more densely populated by particles, showing that the particles migrated toward the core region where the shear rate is lower. From $0.2t_{dev}$ to $0.6t_{dev}$, the most noticeable change is the drop in the number of particles in contact with the wall and the compaction of the suspension in the center of the channel. The color of the particles indicates their streamwise centroid velocity with respect to the mixture bulk velocity. This shows a plug of nearly constant velocity in the channel core, consistent with the high local particle concentration and related suspension viscosity. The core plug becomes thicker over time due to shear-induced particle migration. Outside the plug the particle velocity gradually varies to nearly zero at the walls. Additionally, particle trains are visible where multiple particles are in contact and aligned in an elongated structure. Near the walls, these trains are oriented horizontally as the particles cannot overlap with the wall. Away from the walls, the trains have a predominantly oblique orientation that

is caused by the shear-induced interactions between the particles. Close to the centerline, a tendency for a more horizontal alignment is observed again, caused by the low shear rate and larger solid volume fraction in this region. This indicates a microstructure that changes depending on the wall-normal coordinate, which will be investigated in more detail later.

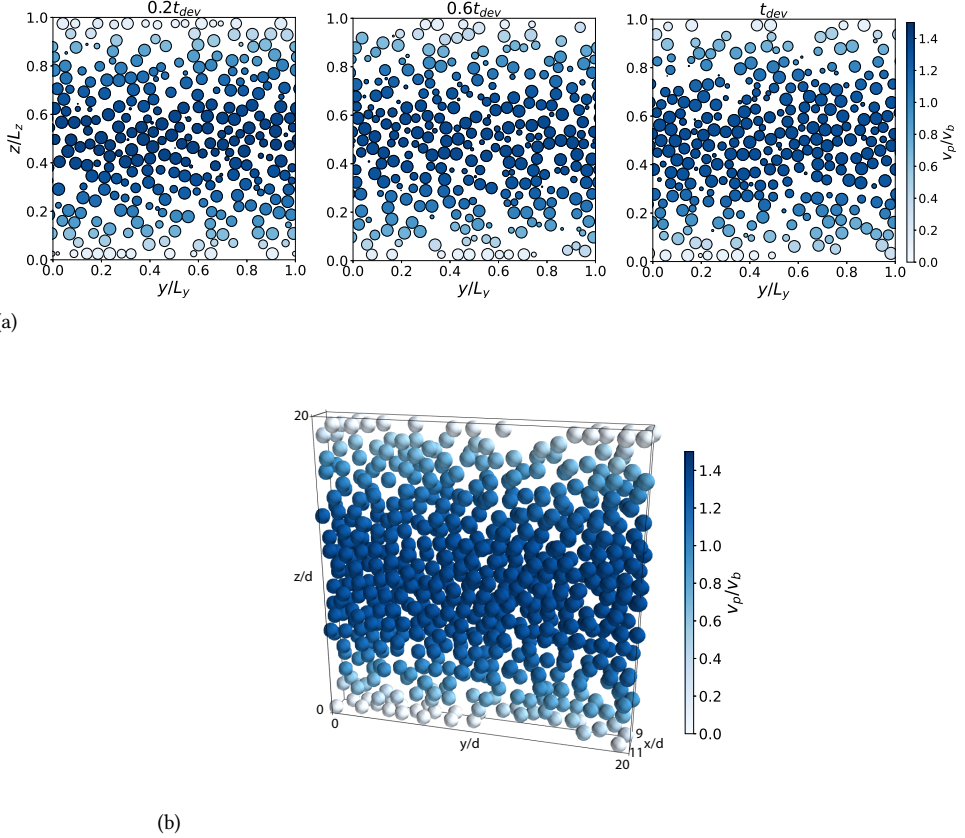


Figure 4.2: (a) Particles in a yz cross-section of the domain at a fixed x -position, shown at three different time instants during the development of the flow for the case with $\phi_b = 0.4$ and $\mu_c = 0$. Time is indicated as a fraction of the development time and particles are colored by their streamwise centroid velocity normalized with the mixture bulk velocity. (b) 3D particle distribution around the cross-section shown in (a) at $t = t_{dev}$.

Using averaging over slabs parallel to the walls, we obtained spatially averaged particle concentration and velocity profiles as a function of the wall-normal coordinate that represent the suspension at a particular time instant. From these profiles, the temporal development of the velocity and concentration profiles can be analyzed. For the cases with $\phi_b = 0.4$, which are used as representative cases to show the results throughout this work, the development of the concentration profile is shown in Figure 4.3 for frictionless (a) and frictional (b) particles. The volume fraction is normalized by the bulk volume fraction. In both cases, there is a distinct particle layer at the wall. At this bulk volume fraction this

layering does not extend into the domain as is the case for higher bulk volume fractions, which will be discussed later. Friction seems to have a pronounced effect on the particles at the wall. In the case with friction, more particles are expelled from the wall layers leading to a lower peak in concentration close to the wall. As seen in the snapshots of Figure 4.2, the particles migrate toward the center. The resulting concentration peak in the core is somewhat steeper for the case with friction; however, the development of the peak and its height are similar in both cases. The development of the profiles is in good qualitative agreement with recent results obtained by Orsi [29] for frictional bidisperse sphere suspensions.

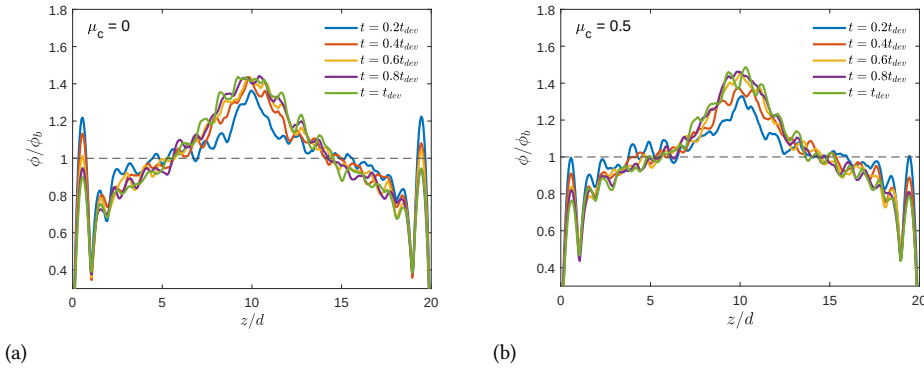


Figure 4.3: Temporal development of the normalized concentration profile, $\phi(y, t)/\phi_b$, for the cases with $\phi_b = 0.4$, and $\mu_c = 0$ (a) and $\mu_c = 0.5$ (b).

To gain more insight into the development of the local solid volume fraction, Figure 4.4 shows the local solid volume fraction as a function of the dimensionless time. Three different locations are shown: (1) $z/d = 0.5$, corresponding to the local concentration peak near the wall in Fig. 3, (2) $z/d = 5$, representative for the intermediate region in between the wall and the channel core, and (3) $z/d = 10$, corresponding to the channel centerline. The vertical dashed line shows the overall development time as determined from the evolution parameter discussed later. These figures show that the particle layer at the wall first becomes more densely populated before the local concentration decreases, which is most pronounced for the case without friction. The local concentration in the intermediate region slightly decreases over time as the result of particle migration toward the core. At the centerline, the volume fraction gradually increases until the maximum value is reached, with a faster development for the case with friction related to stronger shear-induced particle migration. Our results are in good qualitative agreement with the recent work of Orsi [29] for frictional bidisperse sphere suspensions.

The temporal development of the intrinsic fluid velocity profile is shown in Figure 4.5 for the cases with $\phi_b = 0.4$. The velocity profile for single-phase Poiseuille flow is shown by the black dashed line as a reference, which is also the initial condition for the suspension velocity. This profile adapts quickly in the first part of the simulations due to the non-zero particle stress distribution as compared to the single-phase counterpart, followed

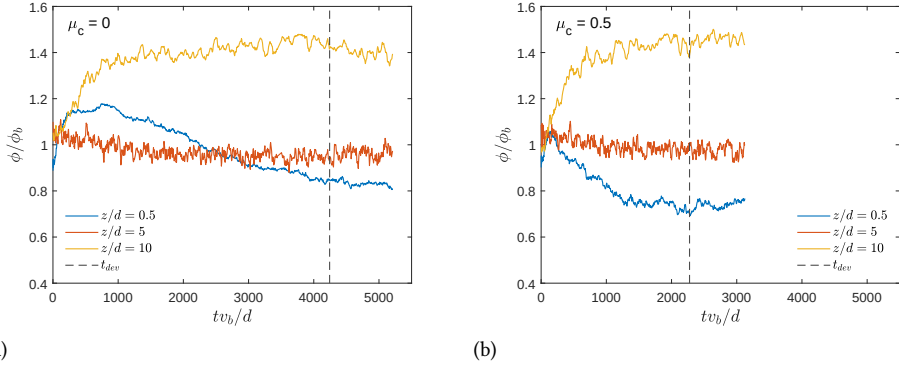


Figure 4.4: Temporal development of the normalized concentration profile, ϕ/ϕ_b , for the cases with $\phi_b = 0.4$, and $\mu_c = 0$ (a) and $\mu_c = 0.5$ (b), shown for three positions in the domain.

by a slow development due to particle migration. The velocity profile for both cases is blunted with respect to the single-phase profile. Looking more closely at the difference between the two cases, it can be seen that up to $0.2t_{dev}$ the case without friction has a slower initial development compared to the case with friction. The blunted profile shows an area in the center of the channel where the velocity gradient is close to zero, indicating a plug flow behavior. In the case with friction, this plug appears to be slightly wider and has a somewhat lower velocity at all times shown here. Furthermore, these figures show that the development of the velocity profile is much quicker than the development of the concentration profile, as the velocity profile hardly changes anymore after $0.6t_{dev}$. The development of the profiles is in good qualitative agreement with recent results obtained by Orsi [29] for frictional bidisperse sphere suspensions.

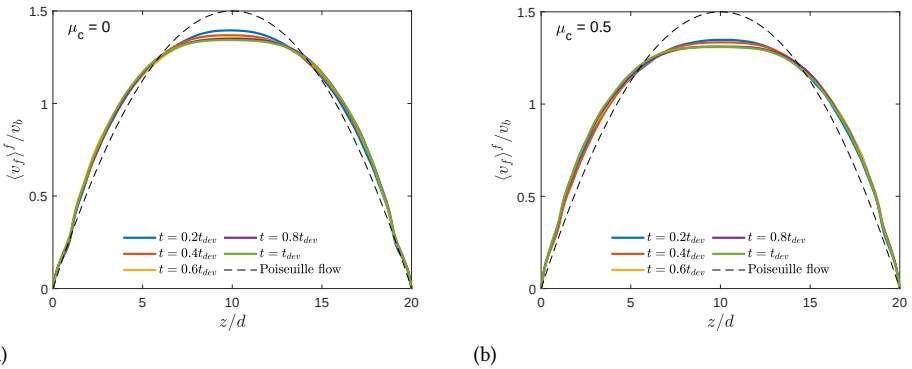


Figure 4.5: Temporal development of the intrinsic fluid velocity profile for the cases with $\phi_b = 0.4$, and $\mu_c = 0$ (a) and $\mu_c = 0.5$ (b).

From the concentration and velocity profiles we observe that the development of the suspension is affected by the friction coefficient. However, we only looked at a single bulk volume concentration so far. To quantify the effect of the bulk concentration and solid friction on the shear-induced particle migration we analyze the time it takes for the suspension to reach a fully developed state. The development time (t_{dev}) can be determined by means of an evolution parameter defined in a similar way as in Hampton et al. [30]:

$$E_p = \frac{1}{L_z} \int \left| \frac{\phi - \phi_b}{\phi_b} \right| dz. \quad (4.22)$$

This evolution parameter measures the deviation of the actual concentration profile from a uniform distribution with a concentration equal to the bulk volume concentration ϕ_b . The evolution parameter can be calculated as a function of time, which is shown in Figure 4.6 for the cases with $\phi_b = 0.4$. To determine the time it takes for the flow to fully develop,

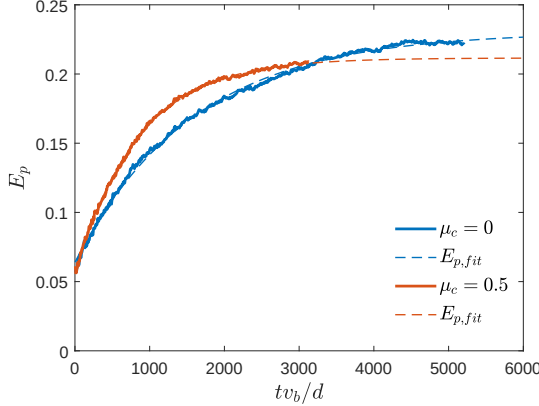


Figure 4.6: Evolution parameter as a function of time for the cases with $\phi_b = 0.4$. Dashed lines show fits of Equation (4.23) to the data.

we fitted a curve to the data of the form:

$$E_{p,fit} = \alpha_1 (1 - e^{-\alpha_2 t}) + \alpha_3, \quad (4.23)$$

where t denotes the time normalized with d/v_b and α_i are the fitting coefficients. The fitted values of α_i are shown in Table 4.2. As can be observed from Figure 4.6, Equation (4.23) provides a very good fit to the temporal evolution of E_p , from which the long-term behavior can be determined even when a simulation is not run until the flow is fully developed. Following Hampton et al. [30], we define the development time as the moment for which the evolution parameter reaches 95% of its long time plateau value $E_{p,\infty} = \alpha_1 + \alpha_3$. The development time is shown in Figure 4.7a as a function of the bulk volume concentration. This shows that the development is faster for the cases with a friction coefficient of $\mu_c = 0.5$ compared to the cases without friction. Furthermore, the development time

Table 4.2: Fitting coefficients for the evolution parameter as defined in Equation (4.23).

μ_c	0				
ϕ_b	0.2	0.3	0.4	0.5	0.6
α_1	0.1732	0.2768	0.1665	0.0831	0.1052
α_2	0.00021	0.00024	0.00063	0.0012	0.0020
α_3	0.0922	0.0592	0.0640	0.0844	0.1045

μ_c	0.5				
ϕ_b	0.2	0.3	0.4	0.5	0.6
α_1	0.1663	0.1876	0.1561	0.0896	0.0385
α_2	0.00024	0.00059	0.0012	0.0023	0.0040
α_3	0.0972	0.0605	0.0555	0.0703	0.0855

appears to decay exponentially with the bulk concentration according to:

$$\frac{t_{dev}}{4H^3/(v_b d^2)} = a e^{-\frac{\phi_b}{\Phi_R}}, \quad (4.24)$$

where $4H^3/(d^2 v_b)$ is used to normalize the development time based on scaling arguments of Nott and Brady [22], a is a dimensionless constant and Φ_R is a reference bulk volume fraction that depends on the Coulomb friction coefficient. Based on a least-squares fit to the data with $\mu_c = 0.5$, we find that $a = 12.5$. Using this value for a , a least-squares fit gives $\Phi_R = 0.165$ for frictionless and $\Phi_R = 0.127$ for frictional particles. For $\phi_b \gtrsim \Phi_R$, t_{dev} drops significantly below the value $t_{dev} \approx 12.5 \cdot 4H^3/(v_b d^2)$ for small ϕ_b . The values found for Φ_R are consistent with the characteristic concentration of roughly 0.1 beyond which particle-particle interactions cannot be ignored anymore and are responsible for the rapid increase in the particle stresses with increasing concentration. As expected, a higher Coulomb friction coefficient corresponds to a lower value of Φ_R , related to faster shear-induced migration due to an enhanced particle stress.

From the development time, the flow development length can be obtained by multiplication with the mixture bulk velocity, $L_{dev} = v_b t_{dev}$. This is normalized with $4H^3/d^2$ [22] and plotted as a function of ϕ_b/Φ_R in Figure 4.7b. Here we also include the analytical expression of Lecampion and Garagash [27] given by Eq. (4.10), the experimental data from Hampton et al. [30] for pipe flow, and the numerical results from Miller and Morris [26] for channel and pipe flow. The corresponding values of Φ_R have been obtained by fitting Eq. (4.24), with $a = 12.5$ fixed, to the data points and are listed in Table 4.3. Following Lecampion and Garagash [33], the development length for pipe flow was multiplied with a factor two for comparison with the channel flow data. Figure 4.7b shows good agreement between the literature data and our numerical results for the range of volume fractions investigated. The analytical expression of Lecampion and Garagash, Eq. (4.10), is in reasonable agreement with the data $2 < \phi_b/\Phi_R < 4$, but large deviations are present

outside this range. Lecampion and Garagash [27] indicate that this discrepancy is caused by the low H/d ratio and low ϕ_b in part of the experiments of Hampton et al. [30] and the related breakdown of the continuum model for the central plug region. However, even for the larger H/d ratio and larger ϕ_b , we see better agreement of the experiments with our fit from Equation (4.24) than with their model. This indicates that the development length for shear-induced particle migration can be described by an exponential decay function in the bulk concentration normalized by an appropriate reference volume fraction. Being able to predict this development length is crucial for the design of experiments or numerical simulations where the aim is to study the steady-state behavior of suspensions in pressure-driven flow. Our scaling indicates that $L_{dev}d^2/(4H^3) = 12.5 \exp(-\phi_b/\Phi_R)$ is solely a function of ϕ_b/Φ_R and implicitly accounts for Coulomb friction through the value of Φ_R . Dependent on the bulk concentration and the Coulomb friction coefficient, the development length may be well over a factor of 100 smaller for dense suspensions near the jamming limit ($\phi_b \approx 0.6$) compared to dilute suspensions for which $\phi_b \ll \Phi_R$.

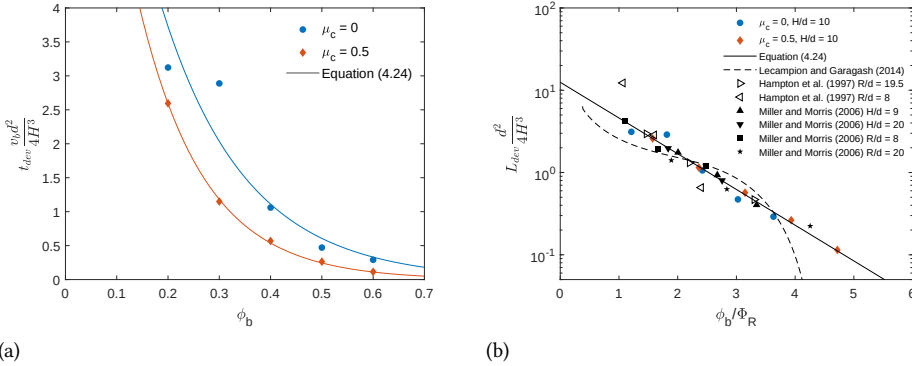


Figure 4.7: Timescale of particle migration as a function of the bulk solid volume fraction (a) and development length as a function of normalized bulk solid volume fraction (b). Development length is compared to the model prediction by Lecampion and Garagash [27] given by Equation (4.10), experimental results from Hampton et al. [30] for pipe flow, and numerical results from Miller and Morris [26] for pipe and channel flow. Following Lecampion and Garagash [27], the development length for pipe flow is rescaled to channel flow according to $L_{dev,channel} = 2L_{dev,pipe}$.

According to the Suspension Balance Model [22, 23, 24], shear-induced particle migration is caused by the divergence of the wall-normal particle stress, which acts as a force that tends to drive the particles in the direction down the gradient in the absolute stress (i.e., in the direction of the channel core). Therefore, we want to see if there is a difference in this stress for the cases with and without friction, explaining the faster development for the cases with friction. Figure 4.8 shows the development of the wall-normal particle stress profiles for the cases with $\phi_b = 0.4$. The stress profiles are averaged over 7 sample fields of the flow around the indicated time spaced 1000 timesteps apart, corresponding to an averaging time of $0.009t_{dev}$ and $0.016t_{dev}$ for the frictionless and frictional case, respectively. This averaging is performed to eliminate the largest fluctuations in the stress profiles for the benefit of showing the mean trend over time. The first clear observation

Table 4.3: Values used for normalization of the solid volume fraction with Φ_R for the different datasets in Figure 4.7b. R denotes the pipe radius in the pipe flow cases.

Dataset	Φ_R
$\mu_c = 0$	0.165
$\mu_c = 0.5$	0.127
Lecampion and Garagash [27]	0.132
Hampton et al. [30] $R/d = 19.5$	0.136
Hampton et al. [30] $R/d = 8$	0.188
Miller and Morris [26] $H/d = 9$	0.150
Miller and Morris [26] $H/d = 20$	0.163
Miller and Morris [26] $R/d = 8$	0.181
Miller and Morris [26] $R/d = 20$	0.106

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is that the magnitude of the wall-normal particle stress is larger for the case with friction. Moreover, the gradients in stress are larger for the case with friction and remain slightly larger when approaching fully developed flow. This would indicate a stronger driving mechanism for migration toward the core for the cases with friction, which is in line with our observation for the development length. The development of the wall-normal particle stress shows good qualitative agreement with the results of Orsi [29] obtained for similar suspensions.

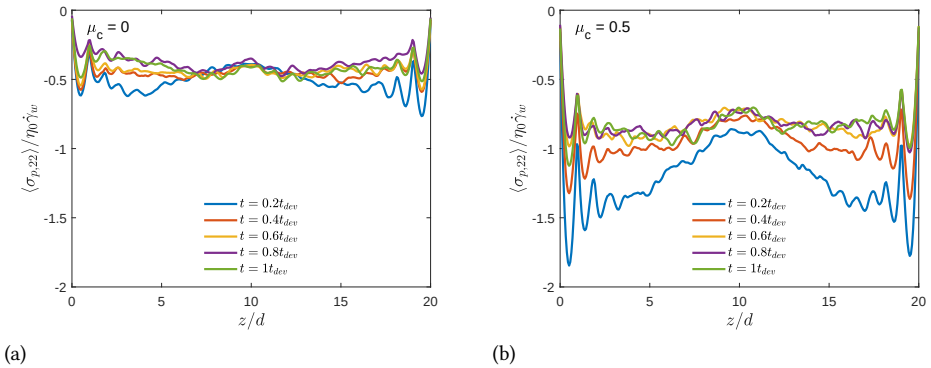


Figure 4.8: Development of the superficial wall-normal particle stress profile over time for the cases with $\phi_b = 0.4$, and $\mu_c = 0$ (a) and $\mu_c = 0.5$ (b). The stress profiles are averaged over 7 sample fields of the flow around the indicated time spaced 1000 timesteps apart, corresponding to an averaging time of $0.009t_{dev}$ and $0.016t_{dev}$ for the frictionless and frictional case, respectively.

4.3.2 Steady-state rheology

Using the development time determined in the previous section, we can define the moment at which the flow reached a statistically steady state in the simulations in order to study the steady-state rheology of the suspension flow. The steady-state statistics presented in this section are obtained by time-averaging of the plane-averaged fields over a time interval $N_{fields}t_{int}$ specified in Table 4.1. This table also specifies which cases are included in the analysis of the steady-state rheology as it was computationally not feasible to run the cases with the lowest volume fractions until the flow was fully developed. The development time increases exponentially for lower bulk volume fraction and/or higher Φ_R , as is clear from Equation (4.24); therefore, we are not able to include the cases with $\phi_b = 0.2$ and the case with $\phi_b = 0.3$ and $\mu_c = 0$.

Steady-state concentration profiles as a function of the wall-normal coordinate are shown in Figure 4.9. In these figures, the concentration is normalized by the bulk concentration for easy comparison between the cases. This shows that the peak in the center of the channel deviates more from the bulk volume fraction for lower values of the bulk volume fraction. Furthermore, we observe a stronger wall-induced layering of particles with increasing bulk volume fraction. This layering extends through the entire channel for the cases with $\phi_b = 0.6$. For $\phi_b = 0.6$ and $\mu_c = 0.5$, there is even a crystal structure visible in the center of the channel, which is different than the layering observed at the wall. The crystal structure in the center of the channel corresponds to a body-centered cubic particle arrangement. This actually resembles the initial particle arrangement with superimposed random perturbations in the particle positions for the cases with $\phi_b > 0.3$, see Section 4.2.2. This shows that at very high bulk concentration, the particles in the channel core do not rearrange but compact into the initial crystal structure. The strong particle layering across the domain severely affects the rheology of the suspensions and is not the focus of the present study. Therefore, we exclude the cases with $\phi_b = 0.6$ from the analysis of the suspension rheology in the remainder of this work.

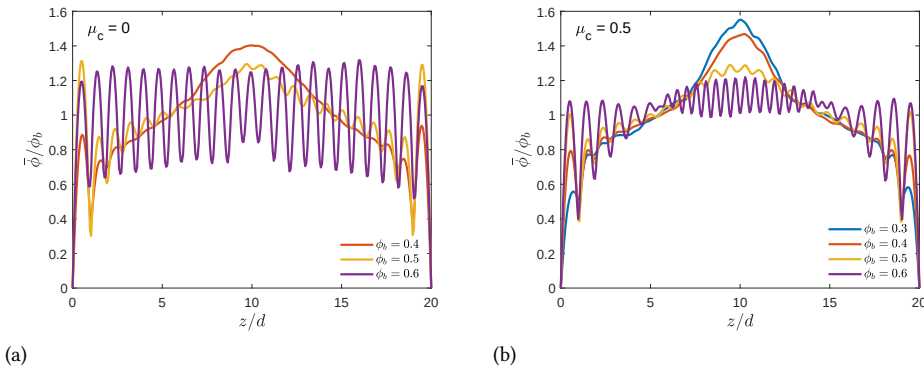


Figure 4.9: Steady-state solid volume fraction $\bar{\phi}/\phi_b$ as a function of the wall-normal coordinate for $\mu_c = 0$ (a) and $\mu_c = 0.5$ (b).

Steady-state velocity profiles for the same cases are shown in Figure 4.10. These figures

show that the velocity profile becomes more blunted and has a lower peak value for higher volume fraction with respect to the parabolic profile for a single-phase flow indicated by the dashed line. The region in the center of the channel, where the velocity gradient is zero, is wider for the cases with friction, showing that these suspensions exhibit a stronger plug flow effect. It is interesting to see that the strong layering for the case with $\phi_b = 0.6$ and $\mu_c = 0$ results in a velocity profile closer to parabolic. This might be because the particle layers can more easily slide past each other resulting in a lower particle shear stress and hence suspension viscosity, as was also observed for strongly layered suspensions in simple shear flow [13].

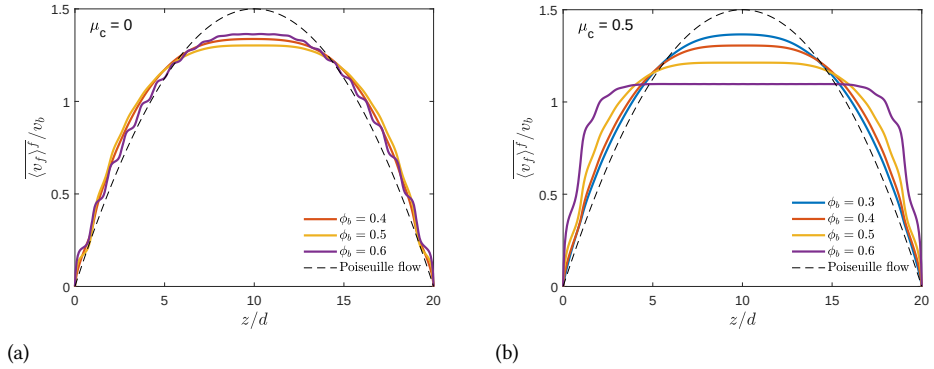


Figure 4.10: Steady-state intrinsic streamwise fluid velocity $\langle v_f \rangle^f / v_b$ as a function of the wall-normal coordinate for $\mu_c = 0$ (a) and $\mu_c = 0.5$ (b).

From the concentration and velocity profiles, three distinct regions in the flow can be distinguished. There is a wall region where particle layering, induced by the flat walls, has a large effect on the local concentration. Moving away from the wall toward the center, there is an intermediate region where wall layering is not present and the intrinsic streamwise velocity increases toward the maximum at the centerline. Finally, in the center of the channel, there is a high local concentration and a constant velocity, which is defined as the core region. To take a closer look at the microstructure of the suspension in these three regions, we have computed the particle pair distribution function (PPDF) defined by:

$$g(\mathbf{r}) = \frac{V/V_{\text{vox}}}{N(N-1)} \sum_p \sum_{p_d} \delta(\mathbf{r} - (\mathbf{x}_{p_d} - \mathbf{x}_p)), \quad (4.25)$$

where V is the total volume of the region of interest, V_{vox} is the voxel volume of the regular voxel grid used for the calculation, N is the total number of particles in the region of interest, $\mathbf{x}_p$ is the centroid position of the reference particle, and $\mathbf{x}_{p_d}$ is the centroid position of a neighboring particle. The function δ gives a value of 1 if the particle centroid of a neighboring particle is in the voxel of interest and 0 otherwise. First, we divide the domain in the three regions mentioned above: the wall region, the core region, and an intermediate region that lies between the two former regions. Based on Figures 4.9 and

4.10, the size of the wall regions is set to three particle diameters from the wall. This is done since wall effects are most pronounced in this region and to ensure that wall effects have minimal effect on the PPDFs of the other two regions. The core region is defined by the plug flow behavior observed in the velocity profiles. The edge of the core region is defined by the position, z_{core} , at which the absolute value of the wall-normal derivative of the plane-averaged streamwise velocity drops below 0.04. This position differs for each case and is therefore determined for all cases separately. An example of the determination of the regions is shown in Appendix 4.A for the case with $\phi_b = 0.4$ and $\mu_c = 0$. The PPDFs of the suspensions are calculated for each region separately, where the PPDF for the wall region has been computed for the reference particle located between $1.25 < z/d < 1.75$, approximately corresponding to the second particle layer from the wall. Due to mirror symmetry in the horizontal mid-plane of the channel, the intermediate and wall region PPDFs are mirrored and averaged over the corresponding regions.

The PPDFs for the case with $\phi_b = 0.4$ and $\mu_c = 0$ are shown in Figure 4.11, where the red color denotes a higher probability of finding a particle at this position, while the blue color denotes a lower probability relative to a statistically homogeneous particle distribution. Note that the colorbar is split at a value of 1, where the parts above and below both scale linearly but with different factors. The pixelated appearance of the figures stems from the voxel resolution used in combination with the finite number of statistically independent samples.

The PPDF of the wall region nicely illustrates what we observed in the concentration profiles of Figure 4.9. By choosing the position of the reference particle in the second layer from the wall, we obtain a clear streak of higher probability at $z/d \approx -1$ corresponding to the layer of particles aligned along the wall. For positive z/d we do not observe layering anymore, as expected from the concentration profile for this case in Figure 4.9a, but we find a higher probability in the compressional quadrant of the flow similar to the intermediate region in Figure 4.11b. The intermediate region shows clear depletion zones along the extensional axis of the flow around the particle, similar to what is observed from PPDFs for simple homogeneous shear flow [46, 13]. Additionally, a lighter streak is visible at a radial position of $r/d \approx 2$ that indicates interactions between multiple particles. This streak is stronger for positive z -coordinates in this figure meaning positions closer to the core of the channel where the suspension is more dense. The PPDF of the core region in Figure 4.11c shows high probability zones close to the particle in both the streamwise direction and the wall-normal direction, indicating that contact occurs mostly in these directions. Furthermore, the locally higher probability at $r/d \approx 2$ extends around the entire particle in this region, consistent with the nearly homogeneous concentration in the central plug region.

A convenient way to compare the shear-plane PPDFs of different cases is to radially average the PPDF over a thin shell between $1 < r/d < 1.05$ around the particle as a function of the azimuthal position of the radius vector. This is shown in Figure 4.12 for all three regions along the surface of the particle in the shear plane. The cases with $\phi_b = 0.6$ are omitted due to strong wall and initial condition effects, as mentioned before. From the results for the wall region, depicted in Figure 4.12a, it is clear that particle layering becomes stronger with increasing bulk volume fraction, which can be seen by the higher

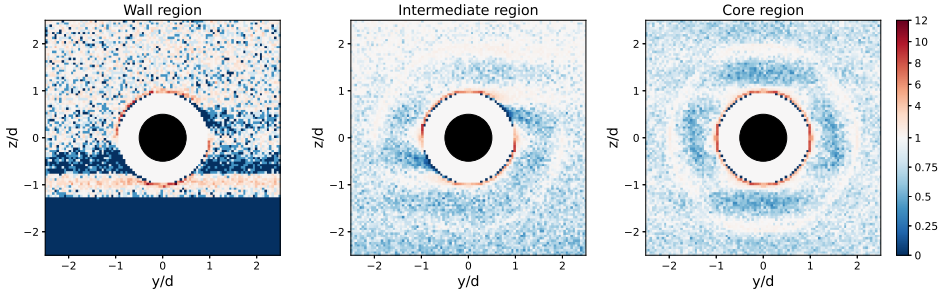


Figure 4.11: Steady-state Particle Pair Distribution Functions (PPDFs) depicted for the shear plane for $\phi_b = 0.4$ and $\mu_c = 0$, shown for the wall (a), intermediate (b) and core region (c). The black circle in the center marks the reference particle. The white area around this marks the excluded volume where no other particle centroids are found as particles do not overlap. For the wall region PPDF, $z/d = -1.25$ marks the location of the wall when the reference particle is located at a distance of $1.25d$ from the wall, therefore $z/d < -1.25$ is colored blue.

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peaks at $\theta = 0, \pi$, and 2π . It seems that the layering starts to become more prominent for $\phi_b > 0.4$, as the results for lower volume fractions show similar behavior. For the cases with $\phi_b = 0.5$, the frictionless case has higher peaks, indicating stronger layering when friction is absent. Common for all cases is a depletion zone around $\theta = 3\pi/4$, which coincides with the extensional quadrant of the flow. If we look at the intermediate region, depicted in Figure 4.12b, the first thing that stands out, is that most lines coincide at $\theta = 3\pi/4$ and $\theta = 7\pi/4$. This marks the edge of the depletion zones in the extensional direction of the shear flow, which is very similar to results obtained for simple shear flow [13]. In the depletion zones it can be seen that increasing bulk volume fraction results in a less low probability. Furthermore, the increase in peak height at $\theta = 0, \pi$, and 2π with bulk volume fraction shows that there is more alignment of particles in the streamwise direction with increasing volume fraction. The effect of friction is not very pronounced in this region, although a slight difference in peak height can be observed, indicating that the frictionless cases exhibit a somewhat stronger alignment in layers. Moving on to the core region, shown in Figure 4.12c, we can see a different structure emerging. The depletion zones are absent, and there is a strong increase in peak height for increasing volume fraction. The absence of depletion zones can be explained by the plug flow behavior that we observed in the velocity profiles, corresponding to a zero mean shear rate in the core. This results in the collective movement of particles with the mean flow, instead of particles moving past each other in layers with different velocities. The higher peaks at $\theta = 0, \pi$, and 2π with increasing bulk volume fraction show that there is stronger alignment of particles in the streamwise direction. There seems to be no difference with regard to friction, indicating that the microstructure is similar in the core region of the flow for frictionless and frictional cases.

From the mean concentration profiles and the suspension microstructure, it becomes evident that the suspensions are not uniformly distributed. This inhomogeneity complicates the calculation of the rheology of the suspensions, because the rheology is dependent on the volume fraction, which changes throughout the channel. Therefore, we study the local rheology of the suspensions in relation to the local volume fraction. To calculate the local

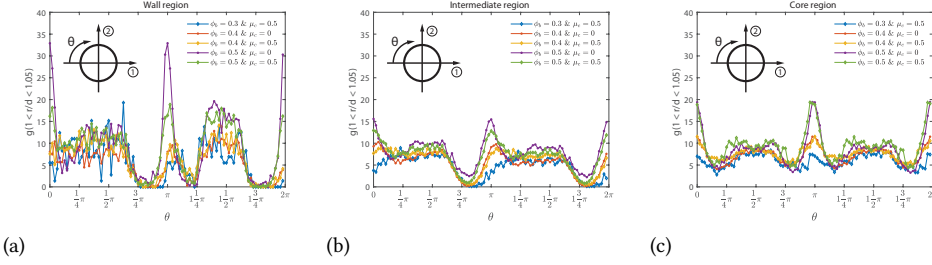


Figure 4.12: Steady-state Particle Pair Distribution Functions (PPDFs) in the shear plane, averaged over a thin shell around the reference particle ($1 < r/d < 1.05$), shown for all cases in the wall (a), intermediate (b), and core (c) regions.

rheology, the stresses as a function of the wall-normal coordinate are required. For the Stokes flow regime, the stress balance for the streamwise direction can be written as (see, e.g., [10]):

$$\frac{1}{Re_b(d/2H)} \frac{\partial \overline{v_m}}{\partial z} + \overline{\langle \sigma_{p,12} \rangle} = (z - z_{core}) \frac{\partial p_e}{\partial y}, \quad (4.26)$$

where the left-hand side is the total shear stress, $\overline{\langle \sigma_{12} \rangle}$, consisting of the viscous and the particle shear stress, respectively, and $\overline{v_m} = \overline{\langle v_f \rangle} + \overline{\langle v_p \rangle}$ is the mean mixture velocity of the suspension. The different stress contributions in this equation are shown in Figure 4.13a as a function of z/d for the case with $\phi_b = 0.4$ and $\mu_c = 0$, where the stress is normalized using the viscous wall shear stress for single-phase Poiseuille flow ($\eta_0 \dot{\gamma}_w$). The total stress coincides with the expected stress determined from the pressure gradient in almost the entire channel, with small deviations close to the wall related to a bias in the reconstruction of the particle stress in a strongly heterogeneous flow, as discussed in Section 4.2.3. The particle stress $\overline{\langle \sigma_{p,12} \rangle}$ has the largest contribution to the total shear stress in this case, in particular in the core region where the particle concentration is highest. As in our previous study on simple shear flows [13], the particle stress can be decomposed into a

hydrodynamic contribution, $\overline{\langle \sigma_{p,12}^{hyd} \rangle}$, and a contact contribution, $\overline{\langle \sigma_{p,12}^{cont} \rangle}$, which are shown by the dashed and dotted line, respectively. Here the lubrication force corrections, discussed in Section 4.2.1, are included in the hydrodynamic contribution of the stress. The hydrodynamic contribution dominates over the contact contribution in the wall region, while the opposite is true for the dense core region where the contact contribution is highest. Contrary to the findings of Yeo and Maxey [37] for frictionless particles, we do neither observe a transition from positive to negative particle shear stress in the core region *below* the channel centerline nor an accompanying sign change in the hydrodynamic contribution; the particle shear stress only changes sign *at* the channel centerline. The reason for the different findings of Yeo and Maxey [37] for the particle shear stress remains puzzling.

The frictional case with $\phi_b = 0.4$ and $\mu_c = 0.5$ is shown in Figure 4.13b. The shear stress shows a small increase in the presence of particle friction for this case. This increase is caused by the increase of the contact contribution of the particle stress, which is still more

or less uniform in the intermediate flow region but has a larger magnitude compared to the case without friction. Looking at the stress balance for the other cases (not shown), we observe a larger magnitude of the total shear stress for higher bulk volume fraction, resulting from a larger contribution of the particle stress component and with a stronger effect in the cases with friction resulting from an increase in the contact contribution. These stress profiles show good qualitative agreement with the results of Orsi [29] for frictional bidisperse suspensions.

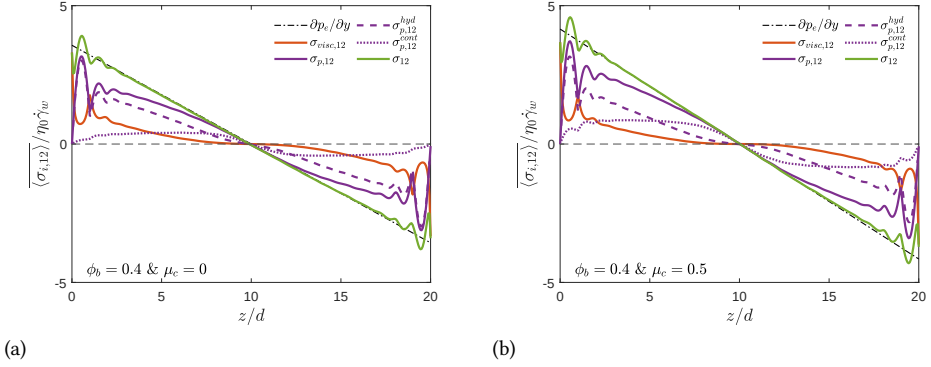


Figure 4.13: Steady-state mean superficial shear stress $\langle \sigma_{i,12} \rangle$ as a function of the wall-normal coordinate for $\phi_b = 0.4$ with $\mu_c = 0$ (a), and $\mu_c = 0.5$ (b). Different colors indicate the various stress terms, while the dashed and the dotted line show the hydrodynamic and the contact contribution to the particle stress, respectively. The dash-dotted line shows the total shear stress distribution expected from the balance with the mean streamwise pressure gradient, $(z - z_{core}) \partial p_e / \partial y$.

From the shear stress balance, we can determine the relative shear viscosity of the suspensions as a function of the wall-normal coordinate. The relative shear viscosity is defined here as the local total shear stress over the local viscous shear stress according to:

$$\frac{\eta}{\eta_0} = 1 + \frac{|\langle \sigma_{p,12} \rangle|}{\frac{1}{Re_b(d/2H)} \left| \frac{\partial v_m}{\partial z} \right|}. \quad (4.27)$$

For the calculation of the relative viscosity, a region of 2 particle diameters wide is excluded near the channel walls, which is affected by the nearby presence of the wall. Additionally, the region where the viscous shear stress becomes close to zero near the centerline is excluded as well. An example of the relative viscosity calculation is shown in Appendix 4.B for the case with $\phi_b = 0.4$ and $\mu_c = 0$. Knowing the relative shear viscosity and the local solid fraction as a function of the wall-normal coordinate, we can combine the two to obtain the relative shear viscosity as a function of the local solid volume fraction. This is shown in Figure 4.14a. This shows that the cases with different bulk volume concentration exhibit similar relative viscosity curves if the local volume fraction is considered. The viscosity diverges at high volume fractions and this divergence occurs at lower local volume fraction for the cases with solid friction. These results are in line with results for the relative

viscosity found in literature for simple shear flows [10, 13]. Looking at the range of local volume fractions observed in each case, we can see a shift to higher local volume fractions with increasing bulk volume fraction. As discussed in the introduction section, it is well known from literature that the relative shear viscosity collapses onto a single curve when the volume fraction is normalized by the maximum flowable packing fraction. To test this for our data, we fitted the Maron-Pierce correlation [19], Equation (4.5), to all data for each friction coefficient to determine the maximum flowable packing fraction. From the results, shown in Figure 4.14b, we observe excellent collapse onto a master curve when the volume fraction is normalized by ϕ_m . The maximum flowable packing fractions are $\phi_m = 0.69$ for the frictionless cases and $\phi_m = 0.62$ for the frictional cases, indicating that the maximum flowable packing fraction decreases with increasing friction coefficient, as expected [13]. These results are in line with results from literature and show that the local relative viscosity in the intermediate regions (i.e., between the core and walls) of pressure-driven channel flow behaves similar to the relative viscosity behavior observed in simple shear flow [13].

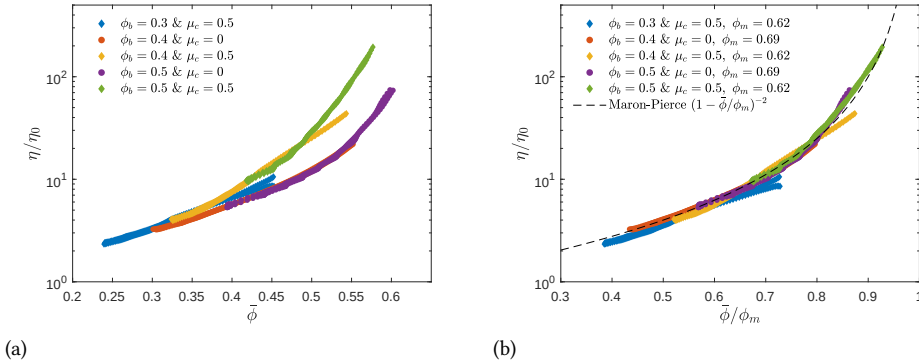


Figure 4.14: Local relative shear viscosity as a function of the local volume fraction (a) and as a function of the local volume fraction normalized by the maximum flowable packing fraction (b). The maximum packing fraction is determined by fitting the Maron-Pierce correlation [19] given by Equation (4.5) to all data with the same Coulomb friction coefficient.

To investigate the divergence of the relative viscosity at large concentration and the effect of friction more closely, the contributions to the total shear stress are separated in the calculation of the viscosity. This results in a hydrodynamic (i.e., the contributions from the viscous stress and the hydrodynamic part of the particle stress) and contact contribution, which are shown in Figure 4.15. The hydrodynamic part coincides for all cases as a function of the local volume fraction as shown in Figure 4.15a, whereas the contact part falls onto two different branches corresponding to the two different values of the solid friction coefficient. When the local volume fraction is normalized by ϕ_m , as done in Figure 4.15b, the hydrodynamic part shows a poorer collapse while the contact part shifts toward a single curve. This shows that the hydrodynamic part scales with the local volume fraction itself, irrespective of the solid friction, whereas the contact part scales with the local

volume fraction normalized with ϕ_m and is strongly affected by solid friction. From this figure, it is also clear that the contacts start to dominate the rheology at a volume fraction of $\bar{\phi}/\phi_m \approx 0.7$, which is in line with previous observations for simple shear flow [13].

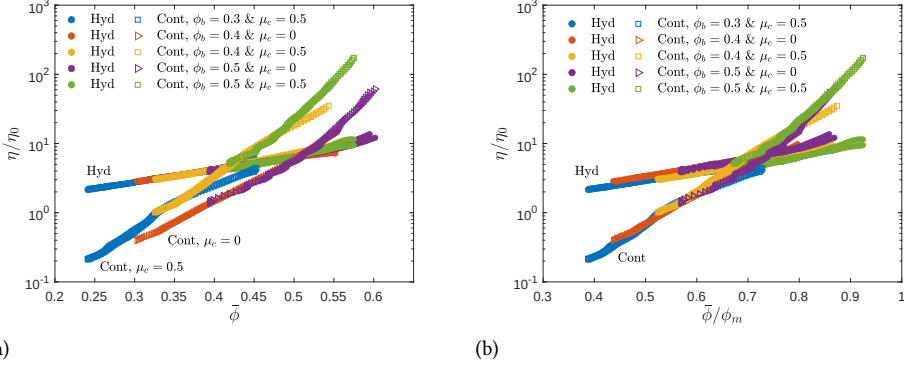


Figure 4.15: Decomposition of the local relative shear viscosity into a hydrodynamic and a contact contribution as a function of the local volume fraction (a) and of the local volume fraction normalized by the maximum flowable packing fraction (b).

To obtain more insight in the suspension rheology, we also studied the normal stresses and in particular the wall-normal stress. The stress balance for the wall-normal direction is written as:

$$-\langle \bar{p} \rangle + \langle \bar{\sigma}_{p,22} \rangle = \text{const.}, \quad (4.28)$$

where the left-hand side represents the total normal stress, $\langle \bar{\sigma}_{22} \rangle$. The fluid pressure is defined relative to the average wall pressure in the simulations, hence $\langle \bar{p} \rangle = 0$ at the walls, and the constant in Equation (4.28) is thus equal to the wall-normal particle stress at the walls. Figure 4.16 shows the pressure and the wall-normal particle stress for the cases with $\phi_b = 0.4$. Here we observe that the total normal stress is constant in the center of the channel, as expected, while oscillations are visible near the walls related to the bias in the reconstruction of the particle stress mentioned before. A more accurate determination of the particle stress at the wall, based on the average particle/wall contact force per unit area, is shown by the black dash-dotted line and shows perfect agreement with the value of the wall-normal stress in the core. The total normal stress is dominated by the contribution from the normal particle stress, while the contribution from the fluid pressure is comparatively smaller in magnitude and has the opposite sign. The decomposition of the particle stress shows that the contact contribution is dominant, while the hydrodynamic part has the opposite sign and is of the same order as the fluid pressure. The magnitude of the total wall-normal stress increases in the presence of solid friction, as shown in Figure 4.16b. This increase is mostly accounted for by an increase in the contact contribution to the particle stress, as observed before for the increase in the total shear stress in the presence of solid friction. Looking at all the cases (not shown), we observe that the magnitude of the wall-normal stress increases with increasing volume fraction and the effect of friction is present for all volume fractions considered here.

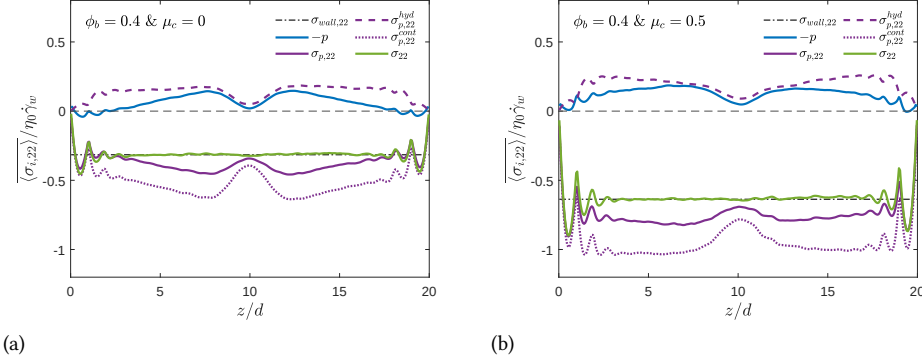


Figure 4.16: Steady-state mean superficial wall-normal stress $\langle \sigma_{i,22} \rangle$ as a function of the wall-normal coordinate for $\phi_0 = 0.4$ with $\mu_c = 0$ (a), and $\mu_c = 0.5$ (b). Different colors indicate the various stress terms, while the dashed and the dotted lines show the hydrodynamic and the contact contribution to the particle stress, respectively. The black dash-dotted line is the wall-normal stress computed from the average particle/wall contact force per unit wall area.

The anisotropy of the microstructure of the suspension induces anisotropy in the normal particle stresses [10], a feature of non-Newtonian behavior. The local normal particle stresses normalized by the local total shear stress are shown in Figure 4.17 for all three directions. Correlations introduced by Badia et al. [47] are fitted to the data and are given by:

$$\frac{\langle \sigma_{p,11} \rangle}{|\langle \sigma_{12} \rangle|} = a_1 \left(\frac{\bar{\phi}}{\phi_m} \right)^{a_2}, \quad (4.29a)$$

$$\frac{\langle \sigma_{p,22} \rangle}{|\langle \sigma_{12} \rangle|} = \frac{\langle \sigma_{p,11} \rangle}{|\langle \sigma_{12} \rangle|} \left(b_1 + b_2 \frac{\bar{\phi}}{\phi_m} + b_3 \left(\frac{\bar{\phi}}{\phi_m} \right)^2 \right), \quad (4.29b)$$

$$\frac{\langle \sigma_{p,33} \rangle}{|\langle \sigma_{12} \rangle|} = \frac{\langle \sigma_{p,11} \rangle}{|\langle \sigma_{12} \rangle|} \left(c_1 + c_2 \frac{\bar{\phi}}{\phi_m} + c_3 \left(\frac{\bar{\phi}}{\phi_m} \right)^4 \right). \quad (4.29c)$$

Here a_i , b_i , and c_i are the fitting coefficients for which the values are shown in Table 4.4. The values for ϕ_m are based on the fit of the Maron-Pierce correlation shown in Figure 4.14b. The correlations are fitted to the data for $\mu_c = 0$ and $\mu_c = 0.5$, which are shown in Figure 4.17 as the dashed and solid black lines, respectively. These fits show a good description of the data with some deviations at high volume fractions. However, the distinction between the two solid friction coefficients is captured well. Figure 4.17d shows the ratios of the normal stress components, $\lambda_2 = \langle \sigma_{p,22} \rangle / \langle \sigma_{p,11} \rangle$ and $\lambda_3 = \langle \sigma_{p,33} \rangle / \langle \sigma_{p,11} \rangle$. These ratios show little dependence on the friction coefficient and more or less collapse to a single curve. Both λ_2 and λ_3 increase with increasing volume fraction, with λ_2 being consistently larger than λ_3 .

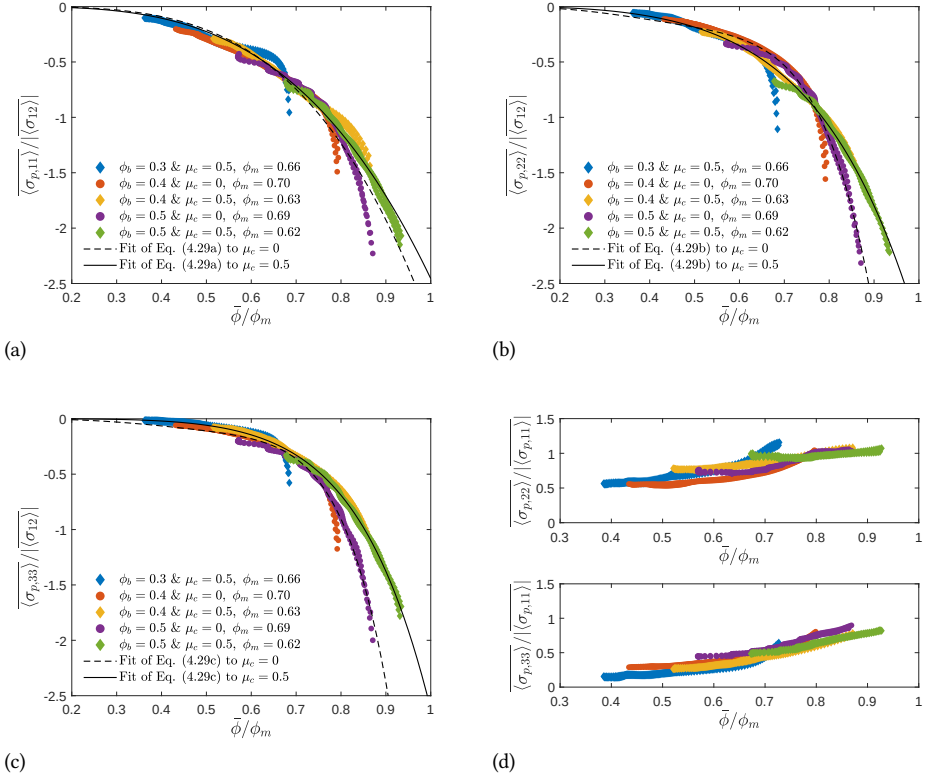


Figure 4.17: Normal particle stresses $\langle \sigma_{p,ii} \rangle$ as a function of the normalized local solid volume fraction in the streamwise (a), wall-normal (b), and spanwise (c) directions, as well as the ratios λ_2 and λ_3 (d). Lines indicate fits of Equation (4.29) to the data with $\mu_c = 0$ (dashed) and with $\mu_c = 0.5$ (solid).

From the normal stresses, the normal stress differences can be determined. These are defined as:

$$N_1 = \overline{\langle \sigma_{p,11} \rangle} - \overline{\langle \sigma_{p,22} \rangle}, \quad (4.30a)$$

$$N_2 = \overline{\langle \sigma_{p,22} \rangle} - \overline{\langle \sigma_{p,33} \rangle}. \quad (4.30b)$$

Figure 4.18 shows the local normal stress differences normalized by the local shear stress as a function of the normalized volume fraction. The data fall on two separate master curves for the two solid friction coefficients. For the first normal stress difference, shown in Figure 4.18a, we observe slightly negative values with an increase at high volume fraction going to positive values. This behavior was also observed for simple shear flow [13], which is shown as the colored dashed lines. The blue dashed line corresponds to simple shear flow of frictionless particles [13] and matches very well with our data. The same holds for the frictional case shown by the red dashed line, even though the friction coefficient is slightly different in those simulations with $\mu_c = 0.39$. From the correlations in

Table 4.4: Fitting coefficients for the correlations describing the normal stresses as defined in Equation (4.29) compared to the coefficients found in previous work on simple shear flows by Peerbooms et al. [13] and by Badia et al. [47].

	DNS		Peerbooms et al. [13]			Badia et al. [47]
	$\mu_c = 0$	$\mu_c = 0.5$	$\mu_c = 0$	$\mu_c = 0.2$	$\mu_c = 0.39$	
a_1	-2.9046	-2.6033	-2.3022	-2.3305	-2.3648	-2.4247
a_2	3.8209	3.7262	2.7915	2.9724	3.0688	4.1280
b_1	5.6457	0.8698	0.9717	0.5938	0.3792	2.1446
b_2	-15.4846	-0.6578	-2.0377	-0.2760	0.4415	-2.7234
b_3	12.0409	0.9583	2.5687	0.9074	0.3524	1.5759
c_1	2.0493	-0.1410	0.5895	0.4977	0.3361	0.3750
c_2	-3.4621	0.6552	-0.5932	-0.3755	-0.0983	0.0366
c_3	3.5545	0.5564	1.8373	1.2661	1.0189	0.4846

Equation (4.29), we can also compute the normal stress differences, shown here by the dashed and solid black lines for frictionless and frictional cases, respectively. These show a somewhat less accurate match with the data compared to the data from simple shear flow, especially for the case without friction. Looking at the second normal stress difference, shown in Figure 4.18b, the distinction between the two friction coefficients is very clear. N_2 is negative with increasing magnitude for increasing volume fraction. The normal stress differences computed from the fits of Equation (4.29) show very good agreement with the data, showing that the correlations for $\langle \sigma_{p,22} \rangle$ and $\langle \sigma_{p,33} \rangle$ are accurate. The lines describing the simple shear flow [13] show good agreement for low volume fractions but show a stronger upswing close to the maximum packing fraction. The dash-dotted line shows a correlation by Badia et al. [47] that was fitted to data compiled from a number of literature sources [7, 48, 49], which matches the general behavior of our data for both normal stress differences quite well.

As discussed in the introduction section, an alternative method to describe the rheology of suspensions was introduced by Boyer et al. [20], in which the so-called viscous number is used as a governing parameter to describe the rheology. We can apply this frictional description of the rheology to pressure-driven channel flow in a similar way as we did for the relative viscosity, by looking at the local values. The viscous number is defined as the local viscous shear stress over the local wall-normal particle stress according to:

$$I_v = \frac{1}{Re_p(d/2H)} \left| \frac{\partial \langle v_m \rangle}{\partial z} \right| \frac{1}{-\langle \sigma_{p,22} \rangle}. \quad (4.31)$$

In this approach, a macroscopic friction coefficient μ is used instead of the shear viscosity of the suspensions. This friction coefficient is defined as the local total shear stress over

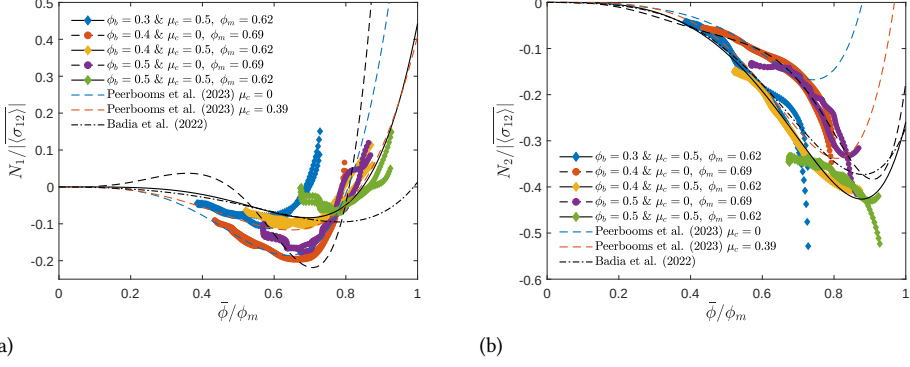


Figure 4.18: First (a) and second (b) normal stress difference as a function of the normalized local solid volume fraction. Black dashed and solid lines show normal stress differences based on fits of Equation (4.29), colored dashed lines are results from Peerbooms et al. [13] for simple shear flow, and the dash-dotted line shows a correlation from Badia et al. [47].

the local wall-normal particle stress according to:

$$\mu = \frac{\frac{1}{Re_b(d/2H)} \left| \frac{\partial \langle v_m \rangle}{\partial z} \right| + \left| \langle \sigma_{p,12} \rangle \right|}{-\langle \sigma_{p,22} \rangle}. \quad (4.32)$$

For the evaluation of the $\mu(I_v)$ rheology, a region near the walls of 2 particle diameters wide is excluded to eliminate wall effects, as we also did before for the evaluation of the relative suspension viscosity. Contrary to the calculation of the relative viscosity, the core of the channel is included for the frictional rheology description because the normal particle stress remains finite (nonzero) throughout the domain.

The macroscopic friction coefficient as a function of the viscous number is shown in Figure 4.19a. This shows that each case describes a viscous number range that shifts toward lower I_v with increasing volume fraction. With this shifting range, the data of the different simulation cases collectively describe a curve similar to the models proposed in literature [20, 7, 40], shown by the black lines. However, there is a deviation from the models at low viscous number for all the cases, corresponding to the core region. For small I_v , $\mu < \mu_1 \approx 0.3$ and the macroscopic friction coefficient is thus lower than the minimum value found for simple shear flows, which is referred to as “subyielding” by Gillissen and Ness [28]. Subyielding starts at lower I_v for higher ϕ_b and higher μ_c , related to a stronger wall-normal particle stress and hence lower I_v at the edges of the core region where the homogeneous shear flow rheology based on the mean shear rate breaks down. The model fitted in our previous work to DNS data for simple shear flow [13], shown by the colored dashed lines, shows a better agreement for high viscous numbers, but follows the same trend as the other models from literature. The colored solid lines show the result from a modified model, which will be discussed later.

Figure 4.19b depicts the normalized local volume fraction as a function of the viscous number. Over the entire range of viscous numbers, the data show a behavior similar to the models in literature [20, 7, 40], with a collapse of the data for high viscous numbers. However, the deviation of our data from the model predictions is also evident here for low viscous number. For the case with $\phi_b = 0.5$ and $\mu_c = 0.5$, $\bar{\phi}/\phi_m = 1.027 > 1$ for small I_v , thus indicating the presence of “overcompaction” [28] in the core. For the other cases shown in Figure 4.19b, the maximum concentration is lower than ϕ_m . This indicates that for lower ϕ_b and/or lower μ_c , shear migration is not strong enough to cause jamming of the suspension flow in the core, contrary to the jamming prediction of the Suspension Balance Model as discussed in the introduction. The modified frictional rheology model of Lecampion and Garagash [27], given by Equations (4.9a) and (4.9b), allows for subyielding and overcompaction, but suffers from the problem that it *always* results in overcompaction in the core region, irrespective of the values for the bulk volume fraction and Coulomb friction coefficient (see, e.g., Fig. 6b in their manuscript).

The scatter at low viscous number in Figures 4.19a and 4.19b, is caused by the dense particle plug in the center of the channel that has developed due to shear-induced particle migration, with a maximum local volume fraction that does not scale with the maximum flowable packing fraction. Inside this plug, the mean shear rate approaches zero at the centerline, decoupling the behavior in the plug from the maximum *flowable* packing fraction ϕ_m that is used to scale the rheology in the model of Boyer et al. [20]. To possibly improve the extension of the homogeneous frictional rheology model to pressure-driven channel flow with heterogeneous shear, we first need to know the cause of the deviation of our data from existing homogeneous shear rheology models. Therefore, similar to the decomposition of the relative shear viscosity shown in Figure 4.15, we decomposed the macroscopic friction coefficient into the hydrodynamic part, μ^h , and the contact part, μ^c , which are shown in Figures 4.19c and 4.19d, respectively. The hydrodynamic contribution shows a very good collapse of the data down to low viscous numbers, where there is a larger spread on the data, but no clear consistent deviation from the existing models; the presence of two different branches in our data points for small I_v is related to a small asymmetry and slight lack of statistical convergence of the flow in the core region. It appears that our data for the hydrodynamic part can be well described by the model of Gallier et al. [7] given by Equation (4.8). The value of ϕ_m used in this model, is based on the Maron-Pierce fit to the relative shear viscosity shown in Figure 4.14b. The fits to the model of Gallier et al. [7] are shown in Figure 4.19c by the dashed and solid black lines (without markers) for $\mu_c = 0$ and $\mu_c = 0.5$, respectively, and show a good description of the data. The model coefficients are shown in Table 4.5.

Looking at the contact contribution in Figure 4.19d, it immediately becomes clear that the deviation from the homogeneous shear rheology at low I_v is caused by a strong decrease in μ^c . Where the contact contribution in simple (homogeneous) shear flow reaches a constant plateau value at low viscous number, which is described in existing models by means of a normalized yield stress μ_1 , this plateau is not visible in our data. The easiest modification we can make, is to eliminate the lower plateau from the homogeneous shear rheology

model of Boyer et al. [20] leading to:

$$\mu^c = \frac{\mu_2^p}{1 + I_0^p/I_v}, \quad (4.33)$$

where the superscript p denotes pressure-driven flow. Fitting this equation to the different simulation cases gives a reasonable description of the data that accounts for the decrease at low I_v and is shown by the colored solid lines in Figure 4.19d. Equation (4.33) captures the behavior of μ well for low I_v and reasonably well for the intermediate I_v range where the transition occurs toward subyielding. The values of the model coefficients, μ_2^p and I_0^p , are given in Table 4.5. Together with the model of Gallier et al. [7] for the hydrodynamic part, our modified model for the contact contribution is able to describe the macroscopic friction coefficient as a function of the viscous number across the entire channel, as shown by the colored solid lines in Figure 4.19a, including subyielding in the core region:

$$\mu = \frac{\mu_2^p}{1 + I_0^p/I_v} + I_v + [\eta]\phi_m I_v^{1-n}. \quad (4.34)$$

Our model predicts that subyielding sets in below a critical viscous number given by:

$$I_v^{sub} \approx \frac{I_0^p}{(\mu_2^p/\mu_1^h - 1)}, \quad (4.35)$$

where μ_1^h denotes the limiting value of μ for small I_v in the case of homogeneous shear flow and where we assumed that the hydrodynamic contribution is negligible for small I_v . Furthermore, for $I_v/I_0^p \ll 1$, subyielding is characterized by an approximately linear relationship for the macroscopic friction coefficient given by:

$$\mu \approx \frac{\mu_2^p}{I_0^p} I_v. \quad (4.36)$$

The fitting parameters I_0^p and μ_2^p vary with the bulk solid volume fraction and the solid friction coefficient. Figure 4.20a shows that I_0^p can be described by an exponential decay as a function of ϕ_b/ϕ_m with a collapse of all cases:

$$I_0^p = a e^{-b(\phi_b/\phi_m)}, \quad (4.37)$$

with $a = 4.62 \cdot 10^3$ and $b = 20.1$ coefficients obtained from a least-squares fit to the data. Figure 4.20b shows that μ_2^p decreases linearly with the bulk solid volume fraction:

$$\mu_2^p = a\phi_b + b, \quad (4.38)$$

with $a = -4.53$ and $b = 2.93$ coefficients obtained from a least-squares fit to the data. Interestingly, we can also describe the centerline value of the solid volume fraction by a linear relation with the bulk solid volume fraction, as shown in Figure 4.20c. A least-squares fit to the data yields:

$$\phi_p = a\phi_b + b, \quad (4.39)$$

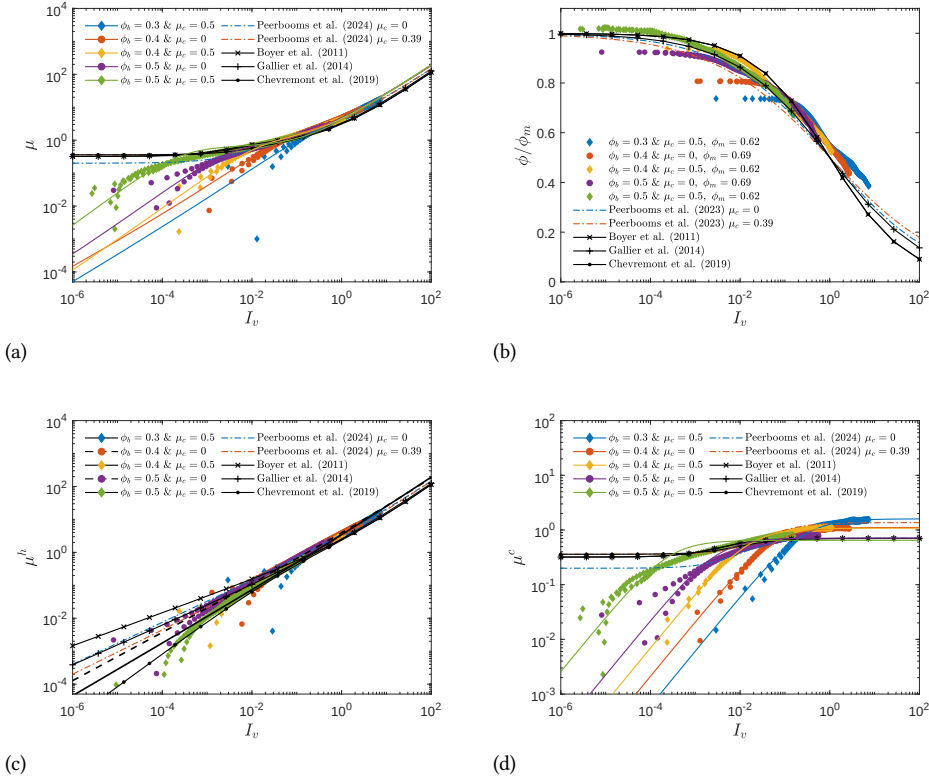


Figure 4.19: Local frictional rheology as a function of the viscous number I_v . (a) Macroscopic friction coefficient μ . (b) Normalized solid volume fraction ϕ/ϕ_m . (c) Hydrodynamic contribution to the macroscopic friction coefficient, μ^h , and (d) contact contribution to the macroscopic friction coefficient, μ^c . Lines show model descriptions as specified in the legends of the figures.

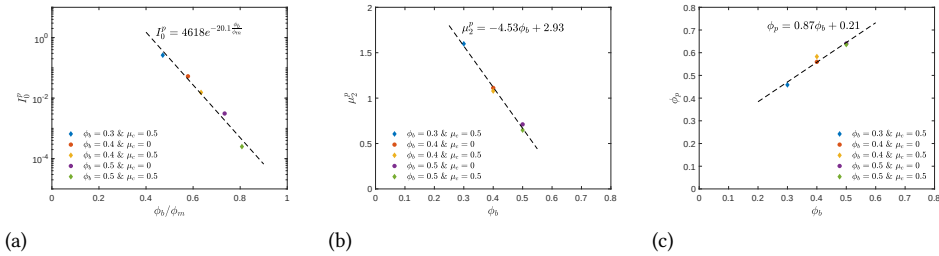


Figure 4.20: Scaling of the fitting parameters. (a) I_0^p and (b) μ_2^p for the modified frictional rheology model and (c) the peak solid volume fraction in the core, ϕ_p .

Table 4.5: Fitting coefficients for the frictional rheology model for pressure-driven channel flow compared to the coefficients for simple shear flow from previous work [13] and literature [20, 7, 40].

	DNS					Peerbooms et al. [13]		
	$\mu_c = 0$		$\mu_c = 0.5$			$\mu_c = 0$	$\mu_c = 0.2$	$\mu_c = 0.39$
ϕ_b	0.4	0.5	0.3	0.4	0.5			
ϕ_m	0.69		0.625			0.72	0.69	0.67
n	0.272		0.209			0.366	0.342	0.331
$[\eta]$	4.27		3.91			3.53	3.27	3.07
μ_1	0	0	0	0	0	0.2	0.3	0.36
μ_2	1.112	0.711	1.598	1.078	0.648	0.71	0.88	1.04
I_0	0.0526	0.0032	0.262	0.0154	2.5e-4	0.0194	0.0368	0.0584

	Boyer et al. [20]	Gallier et al. [7]	Chèvremont et al. [40]
ϕ_b			
ϕ_m	0.585	0.64	$f(\mu_c)$
n	0.5	0.4	0.5
$[\eta]$	2.5	2.4	2.5
μ_1	0.32	0.32	0.36
μ_2	0.7	0.7	0.7
I_0	0.005	0.005	0.0133

where $a = 0.87$ and $b = 0.21$ coefficients obtained from a least-squares fit to the data. Instead of using the bulk volume fraction, we can therefore use Equation (4.39) to express I_0^p as a function of ϕ_p/ϕ_m and ϕ_m and μ_2^p as a function of ϕ_p .

To complete the description of the frictional rheology for pressure-driven channel flow, a relation between the volume fraction and the viscous number is needed. The existing models from literature based on Equation (4.6), with ϕ_m obtained from fitting the Maron-Pierce correlation to the relative shear viscosity data, do not satisfy our data due to the deviation at low I_v , as is clear from Figure 4.19b. Inside the central plug region the local volume fraction is independent of I_v and given by Equation (4.39), while outside the central plug region the model of Boyer et al. [20] for homogeneous shear flow, Equation (4.6), provides a good description of the data. Because the transition to the plateau value is smooth and occurs at different I_v and $\bar{\phi}$ for each simulated case, it is not straightforward to accurately define the edge of the plug from Figure 4.19b. Instead, we turn to the suspension behavior itself to define this transition.

Inside the central plug region, the mean shear rate goes to zero when approaching the centerline, while shear stress fluctuations remain present. This motivates to introduce an ‘rms shear’ viscous number, Θ_v , based on the rms of the fluctuating viscous shear stress with the rms shear rate estimated from the ratio of the square root of the so-called gran-

ular temperature, $\sqrt{T_g}$, and the particle diameter, d ; this proxy is similar to the ‘granular fluidity parameter’ in the study by Zhang and Kamrin [50]. In non-dimensional form, Θ_v is given by:

$$\Theta_v = \frac{\sqrt{T_g}/(Re_b(d/2H))}{-\langle\sigma_{p,22}\rangle}, \quad (4.40a)$$

where it is noted that $\sqrt{T_g}$ is normalized with v_b and $\sigma_{p,22}$ is normalized with $\rho_f v_b^2$. The granular temperature is a measure for the kinetic energy per unit mass of the fluctuating particle motions and defined as:

$$T_g = 0.5(u_{p,rms}^2 + v_{p,rms}^2 + w_{p,rms}^2), \quad (4.40b)$$

where $u_{p,rms}^2 = \overline{(u_p - \langle u_p \rangle)^2}^p$ is the variance of the particle velocity in the x direction, and $v_{p,rms}^2$ and $w_{p,rms}^2$ are the variances in, respectively, the y and the z direction and defined in a similar way. In Figure 4.21a, the ‘rms shear’ viscous number (Θ_v) is plotted as a function of the ‘mean shear’ viscous number (I_v). For sufficiently high I_v , Θ_v increases nearly linearly with I_v , related to stronger particle velocity fluctuations for higher mean shear rate, and is independent of the Coulomb friction coefficient. For small I_v , corresponding to the central core region, Θ_v is constant in I_v , with the constant being smaller for higher ϕ_b and higher μ_c . The plateau value is plotted in Figure 4.21b and appears to decay exponentially as a function of ϕ_b/ϕ_m . Based on Figures 20a and 20b, we model Θ_v according to:

$$\Theta_v = \begin{cases} 0.30(I_v^*)^{0.85} & \text{for } I_v \leq I_v^* \\ 0.30(I_v)^{0.85} & \text{for } I_v \geq I_v^* \end{cases}, \quad (4.41a)$$

where I_v^* is the value of I_v at which Θ_v undergoes a transition from a constant value to a power-law function in I_v . I_v^* is given by:

$$I_v^* = 480.6 e^{-13.4 \frac{\phi_b}{\phi_m}}. \quad (4.41b)$$

Interestingly, I_0^p in the frictional rheology model appears closely related to I_v^* according to:

$$I_0^p = 0.44(I_v^*)^{1.5}. \quad (4.42)$$

Figure 4.22a confirms this correlation, except for the case with $\phi_b = 0.5$ and $\mu_c = 0.5$, which clearly deviates from the trend. In Figure 4.22b, I_v^* and I_v^{sub} from Equation (4.35) are depicted as a function of ϕ_b/ϕ_m . Both I_v^* and I_v^{sub} show the same decaying trend for increasing bulk concentration. I_v^* is roughly a factor 15 larger than I_v^{sub} for $\phi_b = 0.2 - 0.4$, while at $\phi_b = 0.5$ and $\mu_c = 0.5$ they collapse. It is not clear what causes the deviation for the case with $\phi_b = 0.5$ and $\mu_c = 0.5$ in Figures 4.22a and 4.22b, but it might be related to the overcompaction that is observed only for this particular case.

In Figure 4.23, the normalized local mean volume fraction, $\bar{\phi}/\phi_m$, is plotted as a function of Θ_v . Outside the central core region, the data collapse onto a single curve, as expected since both $\bar{\phi}/\phi_m$ and Θ_v scale with I_v here. However, in the central core region, corresponding to the low I_v range in each dataset, the data do clearly not collapse.

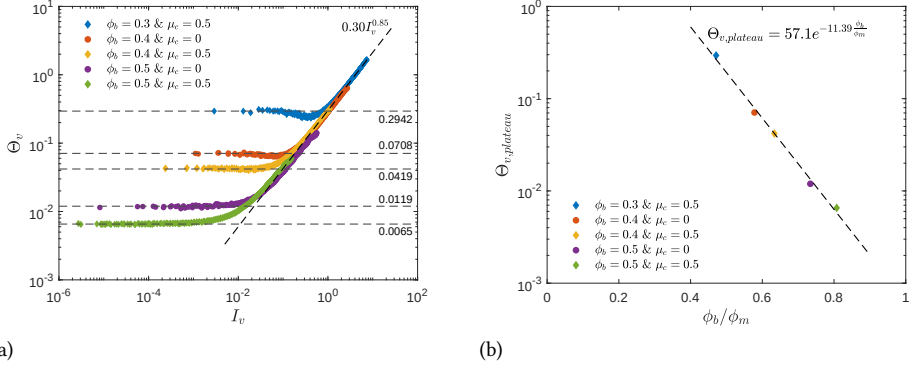


Figure 4.21: (a) Rms shear viscous number, Θ_v , as a function of the mean shear viscous number, I_v , and (b) $\Theta_{v,plateau}$ as a function of ϕ_b/ϕ_m .

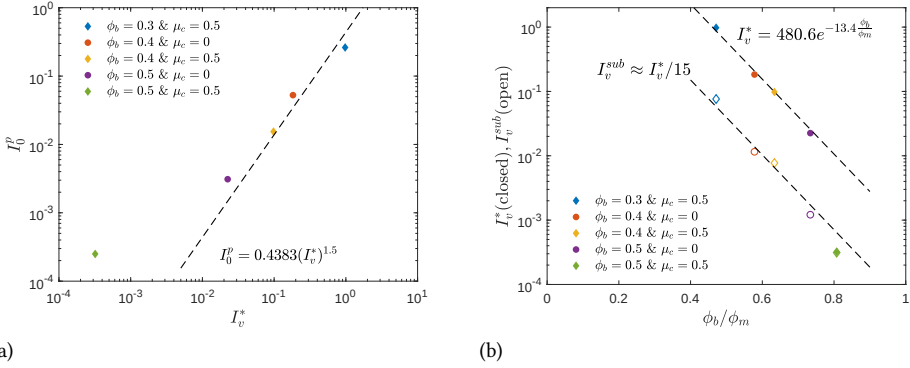


Figure 4.22: (a) I_0^p as a function of I_v^* and (b) I_v^* and I_v^{sub} as a function of ϕ_b/ϕ_m . Note that I_v^* and I_v^{sub} coincide for the case with $\phi_b = 0.5$ and $\mu_c = 0.5$.

Interestingly, we found that the data for the local mean volume fraction can be collapsed by introducing a *modified* maximum flowable packing fraction given by:

$$\phi_{mp} = \phi_p \left(1 - \left(\frac{\Theta_v}{I_v} \right)^q \right) + \phi_m \left(\frac{\Theta_v}{I_v} \right)^q, \quad (4.43)$$

where Θ_v/I_v is a proxy for the ratio of the rms to the mean shear rate and where q is an adjustable parameter. In Figure 4.24, $\bar{\phi}/\phi_{mp}$ is plotted as a function I_v for $q = -0.3$. We find that this value for q yields the best collapse of the data onto a single curve given by Equation (4.6) with ϕ_m replaced by ϕ_{mp} :

$$\bar{\phi} = \frac{\phi_{mp}}{1 + I_v^{0.5}}. \quad (4.44)$$

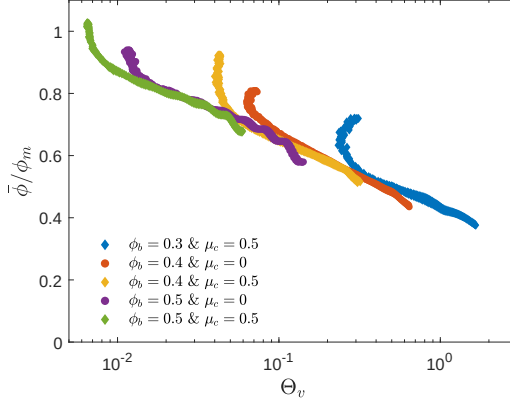


Figure 4.23: Local mean volume fraction normalized with the maximum flowable packing fraction, $\bar{\phi}/\phi_m$, as a function of the 'rms shear' viscous number, Θ_v .

Based on the parameterization of Θ_v as a function of I_v , Equation (4.43) for ϕ_{mp} can be

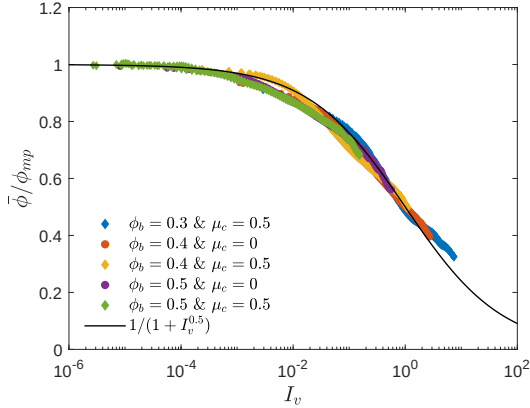


Figure 4.24: Local mean volume fraction normalized with the modified maximum flowable packing fraction, $\bar{\phi}/\phi_{mp}$, as a function of the 'mean shear' viscous number, I_v .

rewritten according to:

$$\phi_{mp} = \begin{cases} \phi_p - 1.44(\phi_p - \phi_m)(I_v^*)^{0.045} \left(\frac{I_v}{I_v^*}\right)^{0.3} & \text{for } \frac{I_v}{I_v^*} \leq 1 \\ \phi_m + (\phi_p - \phi_m)[1 - 1.44I_v^{0.045}] & \text{for } \frac{I_v}{I_v^*} \geq 1 \end{cases} \quad (4.45)$$

In the limit of $I_v/I_v^* \rightarrow 0$, $\phi_{mp} \rightarrow \phi_p$. For $I_v/I_v^* \geq 1$ and $I_v = 1$, $\phi_{mp} \approx \phi_m$ when $\phi_b \approx 0.55$ for $\mu_c = 0$ and when $\phi_b \approx 0.48$ for $\mu_c = 0.5$. It thus appears that $I_v = I_v^*$ marks the transition between the central core region with low mean shear and possible overcompaction (such

as for the case with $\phi_b = 0.5$ and $\mu_c = 0.5$), and the ‘flowable’ region in which the rheology is similar to the rheology for homogeneous shear flows.

4.4 Conclusions

We have presented results from particle-resolved DNS of dense frictionless and frictional suspensions of non-colloidal, monodisperse and neutrally buoyant spheres in viscous pressure-driven channel flow. The channel height was equal to 20 particle diameters. The bulk solid volume fraction was varied in the range of $\phi_b = 0.2 - 0.6$ and two different Coulomb friction coefficients were considered, $\mu_c = 0$ and 0.5 . In our study, we focused on the influence of ϕ_b and μ_c on the flow development and on heterogeneous shear effects on the steady-state rheology. Our main findings are summarized below.

4

Starting from an initially homogeneous particle distribution and the pure fluid flow velocity profile, the particle phase showed shear-induced migration toward the core till equilibrium was reached with a concentration peak at the channel centerline and a blunted mean velocity profile. From the concentration profile, the flow development time, t_{dev} , was determined by introducing an evolution parameter and fitting an exponentially decaying function in time to the data in a similar manner as in Hampton et al. [30]. The development time scales with $H^3/(v_b(d/2)^2)$ and decays exponentially with increasing bulk concentration normalized with a friction-dependent reference concentration, ϕ_b/Φ_R , where $\Phi_R \approx 0.165$ for $\mu_c = 0$ and $\Phi_R \approx 0.127$ for $\mu_c = 0.5$. The reference concentration is interpreted as the bulk concentration beyond which particle contacts are responsible for a rapid increase in the wall-normal particle stress with increasing ϕ_b , resulting in faster shear-induced migration.

At statistically steady state, three distinct regions can be distinguished in the flow: a wall-affected region with a thickness of 2–3 particle diameters and characterized by pronounced particle layering induced by the wall flatness, a dense plug (low-shear) flow region in the core, and an intermediate shear region in which the mean velocity and concentration are gradually increasing from the wall toward the core region. For the highest investigated bulk concentration ($\phi_b = 0.6$), wall-induced layering extended throughout the entire domain, and hence these cases were ignored in the analysis of the suspension rheology. Furthermore, for the lowest investigated bulk concentrations ($\phi_b = 0.2$ & $\phi_b = 0.3$ with $\mu_c = 0$), the flow development time was too long and the simulations had to be stopped before statistical equilibrium was reached. Hence, the steady-state rheology analysis was based only on bulk concentrations in the range of $\phi_b = 0.3 - 0.5$.

Based on the Particle Pair Distribution Function (PPDF), the suspension microstructure in the intermediate region was found to be similar to the PPDFs found for simple (homogeneous) shear flows and characterized by clear depletion zones along the extensional axis of the flow around the particles. These depletion zones are absent in the microstructure in the core region, related to the nearly uniform (low-shear) plug flow here. Furthermore, in the core, the particles preferentially align themselves in the streamwise direction for $\phi \geq 0.4$ without a discernable effect of particle friction, likely related to the collective motion of the particles.

We have analyzed the ‘viscous’ rheology for the intermediate region. In this flow region, the local relative shear viscosity, η/η_0 , scales well with the local concentration normalized with the maximum flowable packing fraction, $\bar{\phi}/\phi_m$, similar to the scaling observed for simple shear flow. Based on fitting the Maron-Pierce correlation to the DNS data, we obtained $\phi_m \approx 0.69$ for $\mu_c = 0$ and $\phi_m \approx 0.62$ for $\mu_c = 0.5$, consistent with the values we previously found for plane Couette flow [13]. The contribution from particle contacts to the relative shear viscosity is dominant beyond $\bar{\phi}/\phi_m \approx 0.7$. The hydrodynamic contribution dominates for smaller volume fractions. This contribution actually scales better with $\bar{\phi}$ rather than $\bar{\phi}/\phi_m$ over the entire range of volume fractions, and is independent of μ_c .

In the intermediate region, the normalized normal stress differences, N_1 and N_2 divided by the local total shear stress, appear to scale fairly well with $\bar{\phi}/\phi_m$, but remain explicitly dependent on μ_c . The results are generally in good agreement with previous results obtained for plane Couette flow [13], though a stronger decrease toward more negative values is observed for high volume fractions in the N_2 data. We also fitted empirical correlations proposed by Badia et al. [47] to the normal stresses, from which the normal stress differences can be fairly well estimated, in particular N_2 . The normal stress anisotropy coefficients, λ_2 and λ_3 , both scale fairly well with $\bar{\phi}/\phi_m$ and show little dependence on μ_c .

We have analyzed the ‘frictional’ rheology for the combination of the intermediate region and the core region. For the higher viscous number (I_v) range, the macroscopic friction coefficient (μ) exhibits similar behavior as in simple shear flow. However, for low I_v , ‘subyielding’ is present with μ decreasing approximately linearly with decreasing I_v at fixed ϕ_b and μ_c . Similarly, for the higher I_v range, $\bar{\phi}/\phi_m$ scales with I_v as in simple shear flow, while for $I_v \rightarrow 0$ the behavior of $\bar{\phi}/\phi_m$ is different from simple shear flow. In the core region, we observed ‘overcompaction’ beyond ϕ_m for the case with $\phi_b = 0.5$ and $\mu_c = 0.5$, while for the other cases at lower ϕ_b and/or $\mu_c = 0$ the maximum core concentration is lower than ϕ_m .

From the decomposition of μ into a hydrodynamic and a contact contribution, we found that subyielding at low I_v originates from a change in the contact contribution with respect to simple shear flow. We presented a modified frictional rheology model that accounts for subyielding in the core region. The macroscopic friction coefficient μ is given by Equation (4.34). Correlations for the model coefficients, I_0^p and μ_2^p , are given by Equations (4.37) and (4.38), respectively. The relation between the local solid volume fraction and the viscous number I_v is described well by Equation (4.44), where ϕ_{mp} is the modified maximum flowable packing fraction defined by Equation (4.43). Based on our results, ϕ_{mp} can be modelled according to Equation (4.45), combined with Equation (4.39) for the maximum core packing fraction, ϕ_p , and Equation (4.41b) for I_v^* . This closes our frictional rheology model for pressure-driven channel flow. This model is able to capture both possible overcompaction in the core region as well as maximum core concentrations below the jamming limit for lower bulk volume fractions.

Compared to frictional rheology models for simple shear flows, key features of the present model for pressure-driven channel flow are: (1) the absence of a yield stress for $I_v \rightarrow 0$, (2) the inclusion of the mean-to-rms shear-rate ratio, I_v/Θ_v , into the model to distinguish between the low-shear plug flow in the core region and the sheared suspension flow in the intermediate region. The transition between the two regions is effectively controlled by

the I_v^* parameter, which represents the value of I_v below which shear-stress fluctuations become decoupled from the local mean shear rate.

In order to validate our proposed frictional rheology model further, a larger range of the Coulomb friction coefficient may be investigated. This would improve the accuracy of the parameterization of the model coefficients. Also, the effects of polydispersity in particle size and shape would be interesting to examine, to be able to model more realistic suspensions in the future. Furthermore, the influence of the particle-to-channel size ratio should be explored further. For the steady-state rheology, we do not expect a strong effect of particle size on the suspension rheology in the intermediate channel region, where the suspension behavior is similar as in homogeneous shear flows. Particle size is expected to have an influence though on wall layering and the central core region as well as on the granular temperature [22].

4

Finally, it would be interesting to use the modified frictional rheology description to improve the Suspension Balance Model (SBM) discussed in the introduction. To compare SBM predictions with the DNS results, still a carefully validated constitutive model for the normal particle stress is required. Our DNS results indicate non-local suspension behavior in the channel core, where the wall-normal particle stress remains nonzero while the ‘mean shear’ viscous number (I_v) approaches zero at the centerline as dictated by statistical flow symmetry. It is precisely for this reason that the classical SBM formulation predicts a peak volume fraction at the channel centerline equal to the maximum flowable packing fraction. Interestingly, our results show that the ‘rms shear’ viscous number (Θ_v) based on the square root of the granular temperature, does remain nonzero, and we proposed a correlation for the plateau value reached in the central core region, see (4.41a). Furthermore, outside the central core region, the rms shear viscous number appears fully correlated with the mean shear viscous number through a power-law relation. These findings support the suggestion of Nott and Brady [22] to base the constitutive relation for the wall-normal particle stress on the fluctuating shear rate, $\sqrt{T_g}/d$, instead of the mean shear rate, $|\partial \bar{v}_m / \partial z|$, or, alternatively, as a function of both. This requires the extension of the SBM with an additional energy equation for the granular temperature. This approach has been shown already to overcome the problem of the classical SBM with the packing fraction at the channel centerline [22]. It is left for future study to explore such constitutive modeling and validation of the SBM in more detail.

Appendix

4.A Example of determination of different flow regions for calculation of the PPDFs

Figure 4.25 shows the determination of the different flow regions in the domain for the calculation of the PPDF for the case with $\phi_b = 0.4$ and $\mu_c = 0$. Figure 4.25a shows the mean intrinsic fluid velocity and its wall-normal derivative. The edge of the core region is defined as the location where $|\partial(\langle v_f \rangle^f / v_b) / \partial(z/d)|$ drops below 0.04. In Figure 4.25b, this region is displayed on the concentration profile, together with the edge of the wall region at three particle diameters from the wall. The intermediate region is defined by $3 \leq z/d \leq z_{core}/d$.

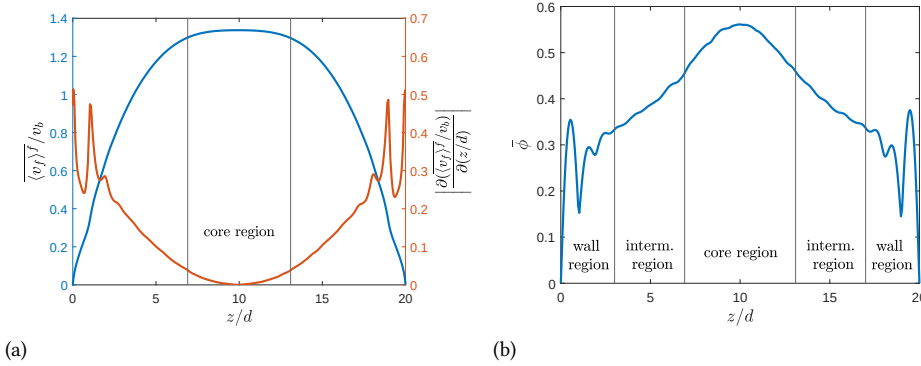


Figure 4.25: Determination of the different flow regions in the domain for calculation of PPDFs for the case with $\phi_b = 0.4$ and $\mu_c = 0$. (a) The mean intrinsic fluid velocity and its wall-normal derivative used to determine the extent of the core region. (b) The mean solid volume concentration as a function of the wall-normal coordinate with the vertical lines delineating the boundaries of the different flow regions.

4.B Example of local relative viscosity calculation

For the case with $\phi_b = 0.4$ and $\mu_c = 0$, Figure 4.26 shows the relative shear viscosity as a function of the wall-normal coordinate for the region considered for the calculation (a) and the corresponding concentration profile in blue with a smoothed profile shown in red (b). The smoothing of the concentration profile is done using a moving average with a width of one particle diameter. This smoothing is also used for the stress profiles in the analysis of the frictional rheology. The region that is excluded near the wall, is 2 particle diameters wide to avoid contamination of the results by wall layering effects. The width of the excluded region in the center of the channel is determined by the local value of the viscous shear stress. The viscous shear stress goes through zero in the center of the channel, causing a singularity in the relative viscosity as can be seen from Equation (4.27).

To avoid this we have chosen to exclude the region where the viscous shear stress drops below a value of $|\langle \sigma_{visc,12} \rangle| / \eta_0 \dot{\gamma}_w < 9e^{-3}$.

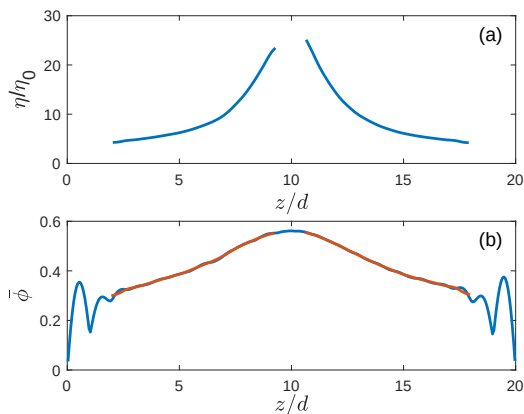


Figure 4.26: Relative shear viscosity as a function of the wall-normal coordinate for the case with $\phi_b = 0.4$ and $\mu_c = 0$, shown for the regions that are included in the calculation (a), and the corresponding concentration profile in blue with a smoothed profile in red for the included regions (b). Smoothing of the concentration profile is done using a moving average with a width of one particle diameter.

References

- [1] Wouter Peerbooms, Antoine van der Heijden, and Wim-Paul Breugem. Transient behavior and steady-state rheology of dense frictional suspensions in pressure-driven channel flow. *Acta Mechanica*, 236(9):5681–5714, 2025.
- [2] Wouter Peerbooms, Antoine E. D. M. van der Heijden, and Wim-Paul Breugem. Data corresponding to the publication: Transient behavior and steady-state rheology of dense frictional suspensions in pressure-driven channel flow. 2024.
- [3] Jonathan J Stickel and Robert L Powell. Fluid mechanics and rheology of dense suspensions. *Annu. Rev. Fluid Mech.*, 37:129–149, 2005.
- [4] Sidhant Pednekar, Jaehun Chun, and Jeffrey F Morris. Bidisperse and polydisperse suspension rheology at large solid fraction. *Journal of Rheology*, 62(2):513–526, 2018.
- [5] Asimina Sierou and John F Brady. Rheology and microstructure in concentrated noncolloidal suspensions. *Journal of Rheology*, 46(5):1031–1056, 2002.
- [6] Ryohei Seto, Romain Mari, Jeffrey F Morris, and Morton M Denn. Discontinuous shear thickening of frictional hard-sphere suspensions. *Physical review letters*, 111(21):218301, 2013.
- [7] Stany Gallier, Elisabeth Lemaire, François Peters, and Laurent Lobry. Rheology of sheared suspensions of rough frictional particles. *Journal of Fluid Mechanics*, 757:514–549, 2014.
- [8] Romain Mari, Ryohei Seto, Jeffrey F Morris, and Morton M Denn. Shear thickening, frictionless and frictional rheologies in non-brownian suspensions. *Journal of Rheology*, 58(6):1693–1724, 2014.
- [9] Abhinendra Singh, Romain Mari, Morton M Denn, and Jeffrey F Morris. A constitutive model for simple shear of dense frictional suspensions. *Journal of Rheology*, 62(2):457–468, 2018.
- [10] Élisabeth Guazzelli and Olivier Pouliquen. Rheology of dense granular suspensions. *Journal of Fluid Mechanics*, 852, 2018.
- [11] Leonardo E Silbert, Deniz Ertas, Gary S Grest, Thomas C Halsey, and Dov Levine. Geometry of frictionless and frictional sphere packings. *Physical Review E*, 65(3):031304, 2002.
- [12] Johanna Fernengel and Olaf Hinrichsen. Influence of material properties on voidage of numerically generated random packed beds. *Chemical Engineering Science*, 233:116406, 2021.
- [13] Wouter Peerbooms, Tim Nadorp, Antoine van der Heijden, and Wim-Paul Breugem. Interparticle friction in sheared dense suspensions: Comparison of the viscous and frictional rheology descriptions. *Journal of Rheology*, 68(2):263–283, 2024.

- [14] Albert Einstein. *Eine neue Bestimmung der Moleküldimensionen*. PhD thesis, ETH Zurich, 1905.
- [15] Albert Einstein. Berichtigung zu meiner arbeit: Eine neue bestimmung der moleküldimensionen. *Annalen der Physik*, 339(3):591–592, 1911.
- [16] GK Batchelor and JT Green. The determination of the bulk stress in a suspension of spherical particles to order c^2 . *Journal of Fluid Mechanics*, 56(3):401–427, 1972.
- [17] Irvin M Krieger and Thomas J Dougherty. A mechanism for non-newtonian flow in suspensions of rigid spheres. *Transactions of the Society of Rheology*, 3(1):137–152, 1959.
- [18] H Eilers. Die viskosität von emulsionen hochviskoser stoffe als funktion der konzentration. *Kolloid-Zeitschrift*, 97(3):313–321, 1941.
- [19] Samuel H Maron and Percy E Pierce. Application of ree-eyring generalized flow theory to suspensions of spherical particles. *Journal of colloid science*, 11(1):80–95, 1956.
- [20] François Boyer, Élisabeth Guazzelli, and Olivier Pouliquen. Unifying suspension and granular rheology. *Physical review letters*, 107(18):188301, 2011.
- [21] David Leighton and Andreas Acrivos. The shear-induced migration of particles in concentrated suspensions. *Journal of Fluid Mechanics*, 181:415–439, 1987.
- [22] Prabhu R Nott and John F Brady. Pressure-driven flow of suspensions: simulation and theory. *Journal of Fluid Mechanics*, 275:157–199, 1994.
- [23] Jeffrey F Morris and Fabienne Boulay. Curvilinear flows of noncolloidal suspensions: The role of normal stresses. *Journal of Rheology*, 43(5):1213–1237, 1999.
- [24] Prabhu R Nott, Elisabeth Guazzelli, and Olivier Pouliquen. The suspension balance model revisited. *Physics of Fluids*, 23(4):043304, 2011.
- [25] Rashid Jamshidi, Jurriaan JJ Gillissen, Panagiota Angeli, and Luca Mazzei. Roles of solid effective stress and fluid-particle interaction force in modeling shear-induced particle migration in non-brownian suspensions. *Physical Review Fluids*, 6(1):014301, 2021.
- [26] Ryan M Miller and Jeffrey F Morris. Normal stress-driven migration and axial development in pressure-driven flow of concentrated suspensions. *Journal of Non-Newtonian Fluid Mechanics*, 135(2-3):149–165, 2006.
- [27] Brice Lecampion and Dmitry I Garagash. Confined flow of suspensions modelled by a frictional rheology. *Journal of Fluid Mechanics*, 759:197–235, 2014.
- [28] Jurriaan JJ Gillissen and Christopher Ness. Modeling the microstructure and stress in dense suspensions under inhomogeneous flow. *Physical Review Letters*, 125(18):184503, 2020.
- [29] Michel Orsi. *Simulation of concentrated non-brownian frictional and adhesive suspensions in linear and nonlinear flows*. PhD thesis, Université Côte d’Azur, 2022.
- [30] RE Hampton, AA Mammoli, AL Graham, N Tetlow, and SA Altobelli. Migration of particles undergoing pressure-driven flow in a circular conduit. *Journal of Rheology*, 41(3):621–640, 1997.

- [31] MK Lyon and LG Leal. An experimental study of the motion of concentrated suspensions in two-dimensional channel flow. Part 1. Monodisperse systems. *Journal of Fluid Mechanics*, 363:25–56, 1998.
- [32] MK Lyon and LG Leal. An experimental study of the motion of concentrated suspensions in two-dimensional channel flow. Part 2. Bidisperse systems. *Journal of Fluid Mechanics*, 363:57–77, 1998.
- [33] C Gao, B Xu, and JF Gilchrist. Mixing and segregation of microspheres in microchannel flows of mono-and bidispersed suspensions. *Physical Review E*, 79(3):036311, 2009.
- [34] C Gao, SD Kulkarni, JF Morris, and JF Gilchrist. Direct investigation of anisotropic suspension structure in pressure-driven flow. *Physical Review E*, 81(4):041403, 2010.
- [35] Sangwon Oh, Yi-qiao Song, Dmitry I Garagash, Brice Lecampion, and Jean Desroches. Pressure-driven suspension flow near jamming. *Physical Review Letters*, 114(8):088301, 2015.
- [36] Ahmadreza Rashedi, Mohammad Sarabian, Mohammadhossein Firouznia, Dallas Roberts, Guillaume Ovarlez, and Sarah Hormozi. Shear-induced migration and axial development of particles in channel flows of non-Brownian suspensions. *AIChE Journal*, 66(12):e17100, 2020.
- [37] Kyongmin Yeo and Martin R Maxey. Numerical simulations of concentrated suspensions of monodisperse particles in a poiseuille flow. *Journal of fluid mechanics*, 682:491–518, 2011.
- [38] Byoungjin Chun, Jin Seok Park, Hyun Wook Jung, and You-Yeon Won. Shear-induced particle migration and segregation in non-brownian bidisperse suspensions under planar poiseuille flow. *Journal of Rheology*, 63(3):437–453, 2019.
- [39] Nathan J Di Vaira, Łukasz Łaniewski-Wollk, Raymond L Johnson, Saiied M Aminossadati, and Christopher R Leonardi. Influence of particle polydispersity on bulk migration and size segregation in channel flows. *Journal of Fluid Mechanics*, 939:A30, 2022.
- [40] William Chèvremont, Bruno Chareyre, and Hugues Bodiguel. Quantitative study of the rheology of frictional suspensions: Influence of friction coefficient in a large range of viscous numbers. *Physical Review Fluids*, 4(6):064302, 2019.
- [41] JF Richardson and WN Zaki. Sedimentation and fluidisation: Part 1. *Trans. Ins. Chem. Eng*, 31:35–53, 1954.
- [42] Wim-Paul Breugem. A second-order accurate immersed boundary method for fully resolved simulations of particle-laden flows. *Journal of Computational Physics*, 231(13):4469–4498, 2012.
- [43] Pedro Costa, Bendiks Jan Boersma, Jerry Westerweel, and Wim-Paul Breugem. Collision model for fully resolved simulations of flows laden with finite-size particles. *Physical Review E*, 92(5):053012, 2015.
- [44] Silvio Tschisgale, Tobias Kempe, and Jochen Fröhlich. A non-iterative immersed boundary method for spherical particles of arbitrary density ratio. *Journal of Computational Physics*, 339:432–452, 2017.

- [45] Francesco Picano, Wim-Paul Breugem, Dhruvaditya Mitra, and Luca Brandt. Shear thickening in non-brownian suspensions: an excluded volume effect. *Physical review letters*, 111(9):098302, 2013.
- [46] Frédéric Blanc, Elisabeth Lemaire, Alain Meunier, and François Peters. Microstructure in sheared non-brownian concentrated suspensions. *Journal of rheology*, 57(1):273–292, 2013.
- [47] Ayoub Badia, Yves D’Angelo, François Peters, and Laurent Lobry. Frame-invariant modeling for non-brownian suspension flows. *Journal of Non-Newtonian Fluid Mechanics*, 309:104904, 2022.
- [48] François Peters, Giovanni Ghigliotti, Stany Gallier, Frédéric Blanc, Elisabeth Lemaire, and Laurent Lobry. Rheology of non-brownian suspensions of rough frictional particles under shear reversal: A numerical study. *Journal of rheology*, 60(4):715–732, 2016.
- [49] Laurent Lobry, Elisabeth Lemaire, Frédéric Blanc, Stany Gallier, and François Peters. Shear thinning in non-brownian suspensions explained by variable friction between particles. *Journal of Fluid Mechanics*, 860:682–710, 2019.
- [50] Qiong Zhang and Ken Kamrin. Microscopic description of the granular fluidity field in nonlocal flow modeling. *Physical Review Letters*, 118(5):058001, 2017.

5

Printability of dense suspensions in Liquid Deposition Modelling

The research outlined in this dissertation was conducted with the goal of improving the understanding of the suspension rheology for the purpose of 3D-printing. The previous chapters show that the rheology of suspensions is complex and many parameters affect the rheology. We focussed completely on the flow inside the printer; however, this is only one part of the process in 3D-printing. The deposition of the materials in complex shapes consisting of multiple layers also puts requirements on the rheology of the materials. In this chapter, we give an overview of the important properties and parameters that need to be considered when looking at the printability of dense suspensions and take a look at methods and models that have been proposed in literature. We evaluate how the outcome of our research can be implemented in these models for the benefit of 3D-printing of dense suspensions for energetic materials. Additionally, we will describe what steps need to be taken to use the results in everyday practice.

The printer that is developed and used at TNO (Netherlands Organization for Applied Scientific Research) to print energetic materials using an extrusion based technique is shown in Figure 5.1. The printer is equipped with two pistons that can push a syringe loaded with the printing suspension. Around the exit of the nozzle, a circular UV-light is placed for direct curing of the extruded material. In the picture, a co-extrusion die is installed, however, the two pistons can also be used side-by-side and equipped with a standard nozzle. The printing method that is employed in this printer can be best described by UV-assisted Liquid Deposition Modelling (UV-LDM)[1]. Standard LDM, without UV-curing, relies heavily on the rheology of the printing liquid. Considering dense suspensions used as the printing liquid, the printability is governed by a number of rheological factors [2, 3]:

- **Yield stress:** a sufficient yield stress is desired to maintain the shape of the filament after deposition, while for some printing methods the yield stress is also necessary to stop outflow at the nozzle when printing is stopped.
- **Shear-thinning behavior:** shear-thinning is desired for flowability of the suspensions, especially when high printing speeds are required the extrusion pressure/force needed increases significantly if the material is not shear-thinning. Additionally, when a contraction is used at the nozzle, the shear rates increase possibly leading to jamming in suspensions that are not shear-thinning.
- **Viscoelasticity:** the suspension should exhibit elastic properties in order to maintain shape after deposition, while the viscous component is important during the flow inside the printer. The shift from elastic to viscous behavior should ideally occur within the window of shear stresses applied during printing.
- **Thixotropic time:** the thixotropic time is important for materials that gain their stability from the build-up of a particle network. These networks are typically broken down when shear is applied, i.e. during printing, and should recover fast enough after deposition to maintain the shape of the filament.
- **Stability:** stability is important for a homogeneous particle distribution. If the particles settle or segregate over time, this inhomogeneity can impact the printing as well as the product performance. Stability is not only important at quiescent conditions but also under flowing conditions.

In the following sections these factors will be used to discuss the assessment of printability in terms of the yield stress, regime maps, the pressure drop, and the suspension stability. Additionally, we will discuss how this applies to the UV-LDM printing method.

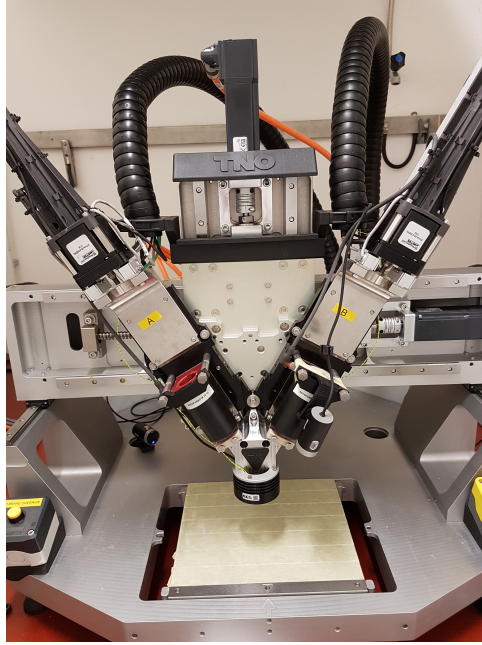


Figure 5.1: Picture of the 3D-printer that is developed and used at TNO to print energetic materials [1].

5.1 Yield stress

These rheological factors indicate that the liquid should be fluid enough to be extrudable through the nozzle, while it should also be rigid enough to maintain its shape after extrusion. To maintain shape after extrusion, the yield stress of the material should be high enough to overcome the force of gravity and capillary forces, trying to deform the filament [4]. A dimensionless number was introduced by M'Barki et al. [4] that shows the balance between these forces:

$$\Xi = \frac{\sigma_y^{Dyn}}{\gamma d_{nozzle}^{-1} + \rho_s g h}, \quad (5.1)$$

where σ_y^{Dyn} is the dynamic yield stress that the material exhibits after cessation of flow, γd_{nozzle}^{-1} corresponds to the stress exerted by surface tension (where γ is the surface tension coefficient and d_{nozzle} the nozzle diameter), and $\rho g h$ denotes the stress due to gravity (where ρ is the density of the material, g the gravitational acceleration and h the typical height of the printed material). Their results showed that, for Boehmite suspensions in deionized water, $\Xi = 1$ indicates a clear limit of printability, as objects printed with $\Xi < 1$ significantly deform after deposition. In order to use this non-dimensional number with our results, we first need to establish a yield stress for the suspensions that we considered. We did not explicitly measure the yield stress, however, the steady-state velocity profiles from Chapter 4 show that we have three different regions of flow behavior. The core of the channel shows a plug flow where the shear is minimal, whereas the flow outside the

core, i.e. in the intermediate and wall regions, shows a varying shear rate. The yield stress can be defined as the total shear stress at the edge of the plug where the shear rate transitions, $\sigma_y^{Dyn} = \sigma_{12}(\dot{\gamma} = \dot{\gamma}_{th})$, where $\dot{\gamma}_{th}$ is a threshold shear rate arbitrarily set to a small value equal to $0.04v_b/d$ to define the edge of the plug region (with v_b the bulk velocity and d the particle diameter). We found that both the total shear stress and the velocity profile are dependent on the bulk solid volume fraction, ϕ_b , and the Coulomb coefficient of sliding friction, μ_c . The resulting yield stresses for all conditions are shown in Figure 5.2 as a function of ϕ_b/ϕ_m and listed Table 5.1. These yield stresses are normalized with the fluid viscosity, η_0 , and the wall shear rate for a Poiseuille flow, $\dot{\gamma}_w = 3v_b/H$ with v_b the bulk velocity and H half of the channel height. From Figure 5.2, we observe that the yield stress as a function of the normalized solid volume fraction can be described using the Maron-Pierce correlation [5],

$$\frac{\sigma_y^{Dyn}}{\eta_0 \dot{\gamma}_w} = \frac{\sigma_{y,0}}{\eta_0 \dot{\gamma}_w} \left(1 - \frac{\phi_b}{\phi_m}\right)^{-2}, \quad (5.2)$$

where $\dot{\gamma}_w$ is the wall shear rate, η_0 the fluid dynamic viscosity, ϕ_b the bulk solid volume fraction, and ϕ_m the maximum flowable packing fraction (varying between 0.625 and 0.69 in our simulations, dependent on Coulomb friction coefficient, μ_c , for particle contacts). This finding is similar to the experimental results of Mahaut et al. [6], where they used the Krieger-Dougherty correlation [7]. From a least-squares fit, we find that $\sigma_{y,0}/\eta_0 \dot{\gamma}_w = 0.15$.

Table 5.1: Yield stress, $\sigma_y^{Dyn}/\eta_0 \dot{\gamma}_w$, determined from the DNS results obtained for pressure-driven channel flow in Chapter 4.

μ_c	ϕ_b	ϕ_m	$\sigma_y^{Dyn}/\eta_0 \dot{\gamma}_w$
0	0.4	0.69	0.95
0	0.5	0.69	2.00
0.5	0.3	0.625	0.56
0.5	0.4	0.625	1.25
0.5	0.5	0.625	3.67

To apply Equation (5.1) to a 3D-printing scenario, incorporating the yield stress we just determined, we need to make the stress dimensional. To calculate a dimensional yield stress, we need to make some assumptions about the printer geometry, the printing conditions, and the suspension properties. If we take an extrusion velocity $v_{ex} = 20$ mm/s though a nozzle with diameter $d_{nozzle} = 2$ mm, and we take into account that the nozzle has a contraction from a tube diameter $d_{tube} = 5$ mm, we find a velocity in the tube of $v_b = v_{ex}(d_{nozzle}/d_{tube})^2 = 3.2$ mm/s. We take a fluid viscosity of $\eta_0 = 10$ Pas and the tube diameter is taken equivalent to the channel height, such that $H = d_{tube}/2 = 2.5$ mm. The resulting $\dot{\gamma}_w = 3.84$ s⁻¹ and the dimensional yield stress in Pa is thus:

$$\sigma_y^{Dyn} = 5.76 \left(1 - \frac{\phi_b}{\phi_m}\right)^{-2} \text{ Pa}. \quad (5.3)$$

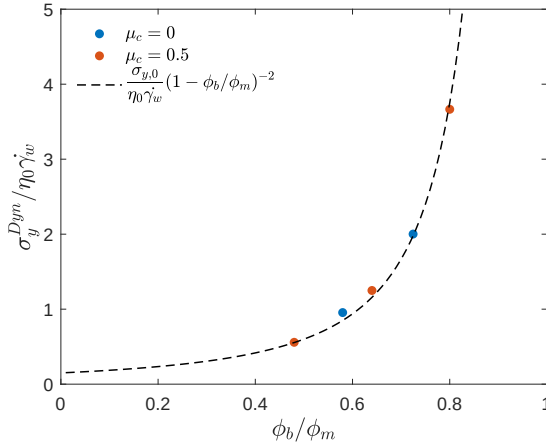


Figure 5.2: Dimensionless yield stress, $\sigma_y^{Dyn}/\eta_0\dot{\gamma}_w$, as a function of the normalized bulk solid volume fraction, ϕ_b/ϕ_m . The markers are based on the DNS results from Chapter 4 and the dashed line gives a fit of Equation (5.2).

The suspension properties are based on the printing application at TNO, where RDX (Research Department Explosive) is used in an acrylate binder. RDX has a density of $\rho_p = 1.8 \text{ g/cm}^3$ and we assume an acrylate binder with a density of $\rho_f = 0.9 \text{ g/cm}^3$ and a surface tension of $\gamma = 70 \text{ mN/m}$. We define the suspension density as $\rho_s = \phi_b\rho_p + (1 - \phi_b)\rho_f$. Using this information we can calculate Ξ as a function of ϕ_b , as shown in Figure 5.3a for $h = 2 \text{ mm}$, the height of the print. For the calculation of the yield stress from Equation (5.3) a value of $\phi_m = 0.625$ is used according to the results obtained for frictional particles in Chapter 4. Figure 5.3a shows that, for the conditions specified above, $\Xi = 1$ for $\phi_b \approx 0.43$, meaning that the extruded filament maintains its shape for suspensions with a solid volume fraction of $\phi_b \gtrsim 0.43$. It is important to note that this value is very much dependent on the assumptions made for the printer geometry, the printing conditions, and the suspension properties. Nevertheless, this exercise shows how valuable a dimensionless number like Ξ can be to determine the printable regime of conditions when the suspension properties and the printing conditions are known. Figure 5.3b shows the contribution of each term in Equation (5.1) as a function of ϕ_b for the case with $h = 2 \text{ mm}$. This shows that the surface tension stress dominates until the yield stress increases strongly for the higher volume fractions. The surface tension dominates due to the small diameter of the extruded filament. If a larger object were considered, the gravitational stress would increase and become dominant over the effect of surface tension.

The evaluation of Ξ for $h = 2 \text{ mm}$ shows that the suspension is printable, in the sense that the filament maintains its shape after extrusion, at $\phi_b/\phi_m > 0.69$. We note that this threshold value for the volume fraction ratio is sensitive to our choice of the threshold value for the shear rate used to define the edge of the plug region in the flow. A lower threshold value for the shear rate will yield a lower estimate of the yield stress and result in a higher estimate of the required bulk solid volume fraction. This might partially explain why our estimate of $\phi_b/\phi_m = 0.69$ is significantly lower than the printable region in the

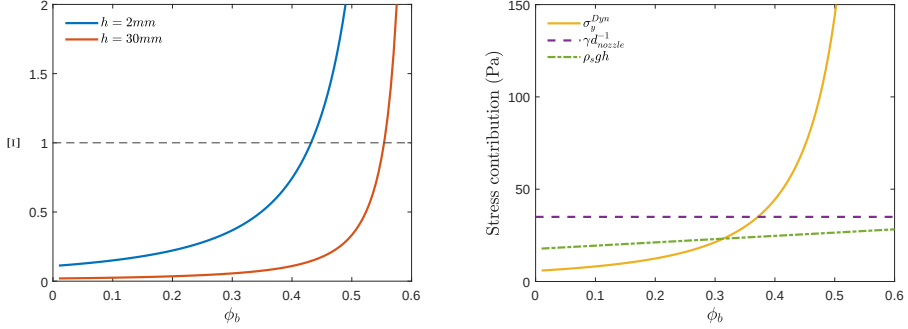


Figure 5.3: (a) Ξ as defined in Equation (5.1) and (b) the separate stress contributions as a function of the bulk solid volume fraction, ϕ_b .

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solid volume fraction that was found by Griebler et al. [8]. They evaluated dense pastes for direct ink writing by small-amplitude oscillatory shear rheometry. They found that the pastes are printable if the solid volume fraction is between $\phi_b/\phi_m = 0.9$ and 0.94. Below this range the suspensions were runny, while above this range the suspensions were jammed. The discrepancy between the results might also be caused by the use of a different metric to determine printability. We looked at the shape retention of a single extruded filament of small diameter, whereas Griebler et al. [8] looked at the slumping of a printed cone of undefined height. To approach the value of $\phi_b/\phi_m = 0.9$ at $\Xi = 1$, we need to increase the print height in our calculation to $h = 30$ mm, as is also shown in Figure 5.3a.

5.2 Regime maps

Another tool that can be used to assess printability in a quick way is a regime map that shows printable regions as a function of rheological parameters. Regime maps for printability of suspensions are typically based on the storage modulus and either the yield stress or the bulk flow stress [9, 10]. In order to use our results for a regime map, some more work needs to be done. The rheology results presented in Chapter 3, are measured at a single shear rate in steady flow conditions. To be able to make the map of bulk flow stress and storage modulus, oscillatory shear flow should be studied. Using our method, the effect of friction coefficient and solid volume fraction on the visco-elastic properties of the suspension can be studied. Together with criteria for printability, for example the criteria summarized by Rau et al. [10], the regimes can be distinguished as a function of the friction coefficient and solid volume fraction. Determining the needed rheological properties can be done by simulating the O.R.O (oscillation-rotation-oscillation) method introduced by Ji et al. [11]. This experimental method enables efficient characterization of dense suspensions by combining various flow conditions in a single test. The alternating blocks of oscillatory and linear shear allow for full characterization of the relevant rheological properties, such as the storage and loss modulus, and thixotropic time.

5.3 Pressure drop

Next to the printability of the suspension itself, the equipment specifications are important for 3D-printing. The force or pressure that is needed to extrude the material can be derived from the rheological properties of the material. The initial pressure difference needed to overcome the yield stress is defined as [12]:

$$\Delta P_{min} = \left(\frac{4L}{D} \right) \sigma_y, \quad (5.4)$$

where L and D are the length and the diameter of the tube, respectively. Our analysis of the yield stress and Figure 5.2 show that this pressure difference will be a function of ϕ_b/ϕ_m and can be described using a Maron-Pierce type correlation. The result of Equation (5.4) is shown in Figure 5.4, using Equation (5.2) to model the yield stress. After overcoming this initial yield stress, the pressure difference needed is lower. The extrusion pressure drop for steady flow can be estimated using the Hagen-Poiseuille equation with the viscosity accounting for the suspension properties [see Eq. (3.219) in Morrison [13]]:

$$\Delta P = \frac{32\eta(\phi_b, \mu_c)LV}{D^2}, \quad (5.5)$$

where V is the bulk velocity and $\eta(\phi_b, \mu_c)$ is the suspension viscosity that is a function of the bulk solid volume fraction and the Coulomb coefficient of sliding friction for particle contacts. Figure 5.4 also shows the pressure drop per unit tube length as a function of the normalized solid volume fraction based on Equation (5.5). This pressure drop is based on the frictional rheology model from Chapter 3, a fluid viscosity $\eta_0 = 1$ Pas, a tube diameter $D = 5$ mm, and an extrusion velocity $v_b = 1$ mm/s. The figure shows that the pressure drop is gradually increasing with volume fraction until it diverges at the approach of the jamming limit.

Equation (5.5) assumes a homogeneous suspension. However, Chapter 4 shows that shear-induced migration leads to heterogeneous particle distributions and the emergence of a plug flow. The development of a plug flow and the resulting velocity profile can be used to obtain a more accurate estimate for the extrusion pressure that is needed for such suspensions. The velocity profile for the region outside the plug flow, can effectively be described by a Power-law model [14, 15] for a shear-thinning fluid¹:

$$\sigma = K \dot{\gamma}^n. \quad (5.6)$$

The fitting was done using a least-squares method and the resulting values for K and n are shown in Table 5.2. Figure 5.5 shows the shear stress as a function of the shear rate from the DNS results of Chapter 4. The solid lines depict the fit of Equation (5.6) to the DNS data. We see that the Power-law model describes the shear stress very well. If we plot the fitting parameters as a function of ϕ_b/ϕ_m , as done in Figure 5.6, we can see that K increases with increasing ϕ_b/ϕ_m , whereas n decreases with increasing ϕ_b/ϕ_m . The latter

¹The origin of the shear-thinning behavior of the suspension is the shear-induced particle migration leading to a gradient in local solid volume fraction. This gradient follows the variation in the shear rate causing the emergence of an apparent shear-thinning, instead of an actual shear-thinning of the fluid.

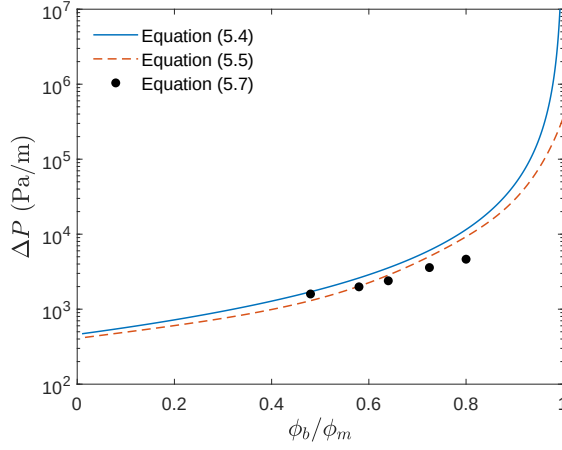


Figure 5.4: Pressure drop per unit length of tube as a function of solid volume fraction, calculated using Equations (5.4), (5.5), and (5.7). We assumed a fluid viscosity $\eta_0 = 1$ Pas, a tube diameter $D = 5$ mm, and an extrusion velocity $v_b = 1$ mm/s.

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shows that the apparent shear-thinning becomes stronger with increasing ϕ_b/ϕ_m . Using the fitted model parameters, the pressure drop per unit length of tube can be determined for each case using [see Eq. (7.92) in Morrison [13]]

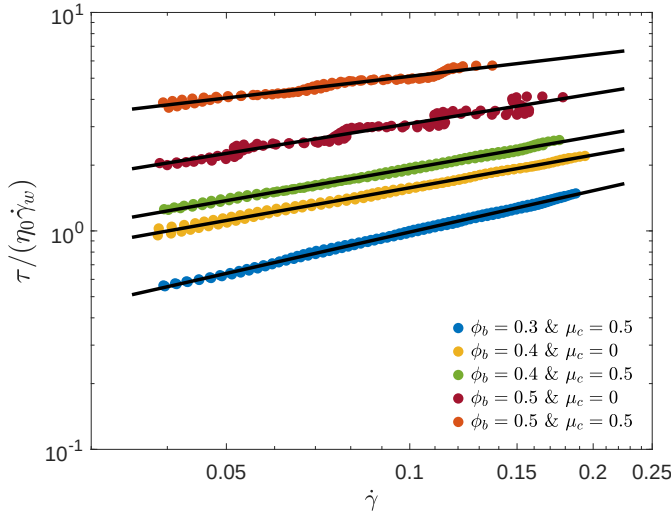
$$\frac{\Delta P}{L} = 2 \left(\frac{3n+1}{n} \right)^n \frac{KQ^n}{\pi^n R^{3n+1}} \text{ Pa/m}, \quad (5.7)$$

where Q is the volumetric flow rate in m^3/s . These values are also given in Table 5.2 and plotted in Figure 5.4. The pressure drop increases with increasing ϕ_b/ϕ_m .

Table 5.2: Values for K and n found by fitting the power-law model to the DNS data from Chapter 4.

μ_c	ϕ_b	K	n	ΔP (Pa/m)
0	0.4	4.96	0.50	1985
0	0.5	8.81	0.45	3587
0.5	0.3	4.21	0.63	1594
0.5	0.4	5.95	0.49	2391
0.5	0.5	10.90	0.33	4637

If we compare Equations (5.4), (5.5), and (5.7) there are some interesting things to note. Equations (5.4) and (5.5) result in very similar curves where the pressure drop based on the Hagen-Poiseuille equation (Equation (5.5)) is slightly lower than the pressure drop based on the yield stress (Equation (5.4)). As expected, the pressure drop diverges at the jamming limit for both results. In contrast, the pressure drop based on the Power-law model (Equation (5.7)) shows a more gradual increase with ϕ_b/ϕ_m . This is caused by the



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Figure 5.5: Shear stress in the intermediate region as a function of the shear rate. Markers indicate the DNS data from Chapter 4 and the solid black lines show the Power-law fit to the data.

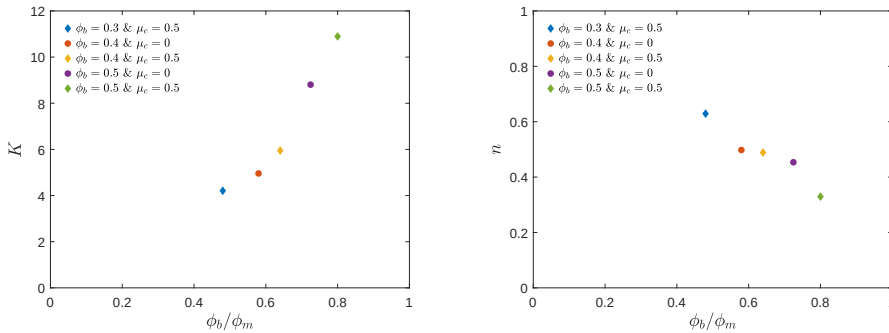


Figure 5.6: Power-law fit parameters (a) K and (b) n as a function of ϕ_b / ϕ_m .

stronger apparent shear-thinning for larger ϕ_b / ϕ_m . The magnitude of the pressure drop for Equation (5.7) is similar to that determined using Equations (5.4) and (5.5) for $\phi_b / \phi_m \approx 0.5$, but due to the more gradual increase the pressure drop is a factor 2.5 lower for $\phi_b / \phi_m = 0.8$. In order to improve the usability of these results, the effect of polydispersity can be incorporated in ϕ_m using the work of Desmond and Weeks [16] and the work of Pednekar et al. [17]. This is useful as monodisperse suspensions, as the ones used in our work, are not common in applications.

5.4 Suspension stability

So far, we have not considered the stability of the suspensions in the above analysis. Stability is defined here in the sense that the particle distribution should remain homogeneous during the printing process. In Chapters 2 and 4 we have seen that the particle distribution tends to deviate from being homogeneous under certain conditions. When the printer is idle the suspension is stationary in narrow tubes, which are usually vertical or at steep angles. Our results show that bulk sedimentation is slow, especially when the tubes are narrow and the solid loading is high. We can use our findings to calculate the distance that a suspension would sediment over time. Let's consider spherical particles with a diameter $d = 250 \mu\text{m}$ and a density $\rho_p = 1.5 \text{ g/cm}^3$. The fluid has a viscosity $\eta_0 = 1 \text{ Pas}$ and a density $\rho_f = 1 \text{ g/cm}^3$. We use the Stokes velocity to determine the settling speed of a single particle in free space and the modified correlation for the sedimentation velocity found in Chapter 2,

$$V_s = k V_0 (1 - \phi_b)^n \left(\frac{1 - \lambda}{1 - 0.475\lambda} \right)^4, \quad (5.8)$$

to calculate the sedimentation velocity of the suspension under the given conditions. With this velocity the sedimentation distance can be plotted as a function of time, as done in Figure 5.7. The effect of solid volume fraction and printing tube diameter are shown in the figure by considering three tube diameters and two bulk volume fractions. The figure

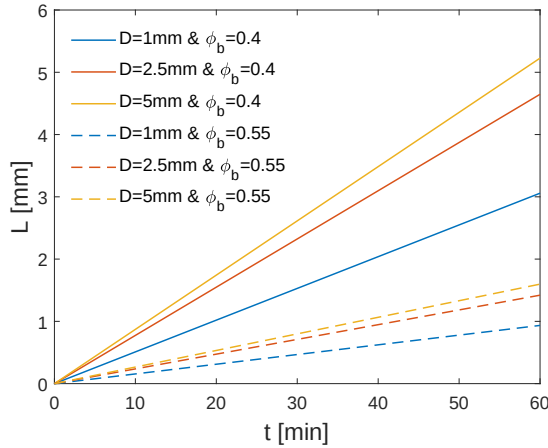


Figure 5.7: Sedimentation distance, L , as a function of the idle time of the printer, t , calculated using Equation (5.8) established in Chapter 2 for a particle diameter $d = 250 \mu\text{m}$, a particle density $\rho_p = 1.5 \text{ g/cm}^3$, a fluid viscosity $\eta_0 = 1 \text{ Pas}$, and a fluid density $\rho_f = 1 \text{ g/cm}^3$.

shows that the distance that the particles travel is only 5 mm, in the worst case considered here, after an hour of the printer being idle. However, in Chapter 2, we have observed inhomogeneity in the microstructure due to particle clustering at much shorter timescales. This could have an effect on the suspension rheology when printing is resumed, but could

also cause practical issues like blocking when a cluster reaches the contraction at the nozzle.

Additionally, we have observed particle migration towards the core of the channel under pressure-driven flow. This creates a variation in solid volume fraction over the radius of the tube. We can use the development time established in Chapter 4 to estimate the length of tube that is needed to reach a fully developed concentration profile. This development length can be written as:

$$L_{dev} = \frac{50D^3}{d^2} e^{-\phi_b/0.127}, \quad (5.9)$$

for frictional particles with $\mu_c = 0.5$. Figure 5.8 shows the development length for the same suspension as above with $d = 250 \mu\text{m}$ and various tube diameters as a function of the bulk volume fraction. We see that, for example, for a suspension with $\phi_b = 0.5$ and a printer with $D = 2.5 \text{ mm}$ a length of tube of 25 cm is long enough for complete particle migration. For very narrow tubes (with respect to the particle diameter) and higher volume fractions the migration happens over even shorter distances. It is important to note that this length scale gives the fully developed concentration profile, while the inhomogeneity already starts at shorter lengths. In Chapter 4, we observed that the centerline concentration already reaches $1.4\phi_b$ at approximately $0.25L_{dev}$, indicating that inhomogeneity due to shear-induced migration sets in quickly.

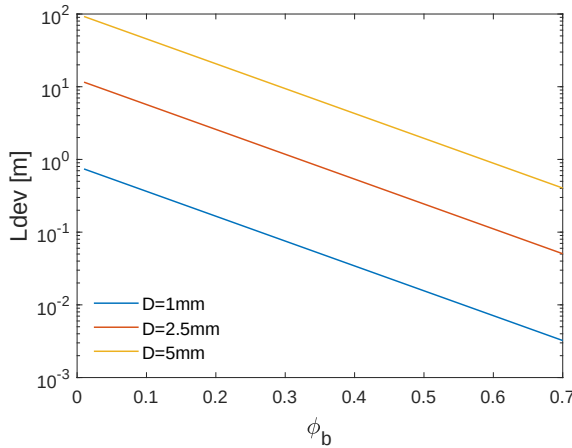


Figure 5.8: Length of tube needed for complete shear-induced particle migration, L_{dev} in Equation (5.9), as a function of the bulk solid volume fraction, ϕ_b , assuming a particle diameter of $d = 250 \mu\text{m}$.

5.5 Application to UV-LDM

If we consider the application that is used at TNO for the 3D-printing of energetic materials using dense suspensions, UV-curing resins are used as a binder material. This enables the use of a UV-light source to start polymerization of the matrix directly after extrusion,

solidifying the material. This could be incorporated in a non-dimensional number, such as Ξ in Equation (5.1), by an additional term in the numerator that takes into account the strength of the solid binder parts. Such a modification might be done as such:

$$\Xi_{UV} = \frac{(1 - C)\sigma_{y,s} + C\sigma_{y,UV}}{\gamma R^{-1} + \rho_s g h}, \quad (5.10)$$

where C is the curing fraction, $\sigma_{y,s}$ is the suspension yield stress, and $\sigma_{y,UV}$ is the yield stress of the UV-cured binder. The literature shows that this binder yield stress is a function of the light intensity and the curing time [18]. Solidification by polymerization softens the criteria for the suspension rheology on dynamic yield stress, elasticity, and thixotropic time to maintain shape after extrusion. However, due to the very high loading required for this application, the criteria on static yield stress and shear-thinning behavior are more stringent to keep the material extrudable. This underlines that a good understanding of the parameters affecting the rheology of dense suspensions is key to develop both equipment and formulations for 3D-printing.

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5.6 Concluding remarks

The rheological factors affecting the printability of dense suspensions discussed in this chapter show that the printability should be assessed for the complete printing process. In the literature, the slumping or dimensional stability of a printed part is often considered. However, our work shows that the flow inside the printer has a large impact on the rheology, and therefore on the printability, of dense suspensions. As discussed in this chapter, more work needs to be done to translate our findings to a comprehensive assessment of the printability, in terms of for instance a regime map. Nevertheless, the insight from our DNS simulations can be used as input for rheological modelling of some of the most important factors in 3D-printing of suspensions, as shown in this chapter for the yield stress, shear-thinning behavior, and suspension stability.

References

- [1] Joost van Lingen. Gradient additive manufacturing of energetics research (gamer). *Netherlands Organisation for Applied Scientific Research*, 2022.
- [2] Peiran Wei, Ciera Cipriani, Chia-Min Hsieh, Krutarth Kamani, Simon Rogers, and Emily Pentzer. Go with the flow: Rheological requirements for direct ink write printability. *Journal of Applied Physics*, 134(10), 2023.
- [3] Alexandra Marnot, Katie Koube, Sungwoo Jang, Naresh Thadhani, Josh Kacher, and Blair Brettmann. Material extrusion additive manufacturing of high particle loaded suspensions: a review of materials, processes and challenges. *Virtual and Physical Prototyping*, 18(1):e2279149, 2023.
- [4] Amin M'barki, Lydéric Bocquet, and Adam Stevenson. Linking rheology and printability for dense and strong ceramics by direct ink writing. *Scientific reports*, 7(1):6017, 2017.
- [5] Samuel H Maron and Percy E Pierce. Application of ree-eyring generalized flow theory to suspensions of spherical particles. *Journal of colloid science*, 11(1):80–95, 1956.
- [6] Fabien Mahaut, Xavier Chateau, Philippe Coussot, and Guillaume Ovarlez. Yield stress and elastic modulus of suspensions of noncolloidal particles in yield stress fluids. *Journal of Rheology*, 52(1):287–313, 2008.
- [7] Irvin M Krieger and Thomas J Dougherty. A mechanism for non-newtonian flow in suspensions of rigid spheres. *Transactions of the Society of Rheology*, 3(1):137–152, 1959.
- [8] James J Griebler, Alexander S Tappan, Simon A Rogers, Jessica W Kopatz, and Anne M Grillet. Methodology to determine printability criteria of highly concentrated pastes through rheological characterization. *Additive Manufacturing*, 96:104578, 2024.
- [9] Esther García-Tuñón, Rishav Agrawal, Bin Ling, and David JC Dennis. Fourier-transform rheology and printability maps of complex fluids for three-dimensional printing. *Physics of Fluids*, 35(1), 2023.
- [10] Daniel A Rau, Christopher B Williams, and Michael J Bortner. Rheology and printability: A survey of critical relationships for direct ink write materials design. *Progress in Materials Science*, 140:101188, 2023.
- [11] Haohao Ji, Jin Zhao, Jie Chen, Shunzo Shimai, Jian Zhang, Yu Liu, Dianzi Liu, and Shiwei Wang. A novel experimental approach to quantitatively evaluate the printability of inks in 3d printing using two criteria. *Additive Manufacturing*, 55:102846, 2022.

- [12] Michael Sweeney, Loudon L Campbell, Jeff Hanson, Michelle L Pantoya, and Gordon F Christopher. Characterizing the feasibility of processing wet granular materials to improve rheology for 3d printing. *Journal of Materials Science*, 52:13040–13053, 2017.
- [13] Faith A. Morrison. *Understanding Rheology*. Topics in Chemical Engineering. Oxford University Press, New York, 2001.
- [14] Armand de Waele. Viscometry and plastometry. *Journal of the Oil and Colour Chemists' Association*, 6:33–69, 1923.
- [15] Wilhelm Ostwald. Über die geschwindigkeitsfunktion der viskosität disperser systeme. i. *Kolloid-Zeitschrift*, 36(2):99–117, 1925.
- [16] Kenneth W Desmond and Eric R Weeks. Influence of particle size distribution on random close packing of spheres. *Physical Review E*, 90(2):022204, 2014.
- [17] Sidhant Pednekar, Jaehun Chun, and Jeffrey F Morris. Bidisperse and polydisperse suspension rheology at large solid fraction. *Journal of Rheology*, 62(2):513–526, 2018.
- [18] Rosaria Anastasio, Wouter Peerbooms, Ruth Cardinaels, and LCA Van Breemen. Characterization of ultraviolet-cured methacrylate networks: from photopolymerization to ultimate mechanical properties. *Macromolecules*, 52(23):9220–9231, 2019.

6

Conclusions and Recommendations

In this chapter we revisit the research questions posed in Chapter 1. These questions have been addressed in several chapters in this work and we highlight the main findings and conclusions. This shows that the rheology of dense suspensions is very complex and more work can be done to improve the understanding of this topic. Therefore, we also describe a number of recommendations to continue and expand on the results that we obtained.

6.1 Conclusions

The goal of this research was to gain more insight into and to improve modelling of the rheology of dense suspensions for the application in UV-assisted Liquid Deposition Modelling. The stages in the printing process that we focussed on were: (1) stationary suspension in the reservoir and tubes of the printer, and (2) suspension flowing through the tubes of the printer. For stage (1), we simulated dense suspensions settling under the action of gravity in narrow vertical tubes, varying the solid volume concentration and the tube-to-particle diameter ratio. For stage (2), we simulated simple shear flow and pressure-driven flow between two parallel plates, varying the solid volume concentration and Coulomb coefficient of sliding friction. Using these simulations, we gained more into the suspension dynamics and rheology in order to answer the following research questions:

What is the effect of the tube-to-particle diameter ratio on the sedimentation dynamics in a viscous fluid?

In Chapter 2, we considered the sedimentation of suspensions in narrow vertical tubes in the viscous regime. Single particle simulations showed that the effect of the tube-to-particle diameter ratio, D/d , can be described very well using the Francis correlation [1]. For suspensions, the effect of the volume concentration on the mean sedimentation velocity is described well by the Richardson and Zaki correlation [2], but modified to include a prefactor k and replacing the terminal velocity of a single settling particle in free space by the Francis correlation [1]. We found $k \approx 0.78$, close to $k = 0.8$ experimentally determined by Di Felice and Parodi [3]. Furthermore, we found $n \approx 4.12$ for the exponent of the hindered settling function, which matches well with the value of $n \approx 4.2$ reported by Yin and Koch [4] for their case with $Ga = \sqrt{20.8}$. Furthermore, we find a scaling relation for the rms velocity normalized by the mean sedimentation velocity of the form $C\phi_b^{1/3}(D/d)^{2/3}$, where $C \approx 0.28, 0.125$, and 0.15 for the vertical, radial, and azimuthal directions, respectively. For the velocity fluctuations, there is a deviation from the trend for $D/(d\phi_b^{-1/3}) \lesssim 2.5$, indicating a change in dynamics for a very small tube-to-particle diameter ratio resulting from very strong confinement. The temporal autocorrelation of the particle velocity shows clear scaling behavior with Equations (2.16a), (2.16b), and (2.16c), for the vertical, radial, and azimuthal directions, respectively. From the rms velocities and the temporal correlations, we determined the Lagrangian length scale of correlated particle motions. The Lagrangian length scale follows the scaling relations defined in Equations (2.17a), (2.17b), and (2.17c), for the vertical, radial, and azimuthal directions, respectively. Where the scaling in the axial and the radial direction do solely depend on the tube diameter and the concentration, while there is also a weak dependence on the particle diameter in the azimuthal direction. We observed vertical concentration heterogeneity in horizontal plane averages, which shows that there is a strong tendency for clustering in the narrow tubes, reminiscent of vertically propagating kinematic waves. The clusters become smaller and less persistent with increasing tube-to-particle diameter ratio, which means that the clusters form and break up over smaller timescales. Our evaluation of the results showed that the dynamics are governed by the local concentration for narrow tubes, while this is not the case for wider tubes. We observed that, for $D/d = 2$, the settling velocity decreases with increasing local volume fraction. For $D/d = 4$, the dependence of the velocity on the

local volume fraction seems to change with bulk volume fraction, whereas, for $D/d \geq 6$, the settling velocity only has a very weak dependence on the local volume fraction. The radial particle distribution also shows heterogeneity, where the wall-region shows peaks in concentration due to an excluded volume effect. Combining this with the radial velocity distribution shows that the particles at the wall sediment slower than the mean, whereas the internal concentration peak corresponds to a maximum in sedimentation velocity for $D/d \geq 4$ and $\phi_b \geq 0.2$. This might correspond to a stable streaming-like pattern where the dense clusters around this concentration peak fall faster than the more dilute core region.

How does solid (interparticle) friction affect the rheology in simple shear flow?

In Chapter 3, we studied the suspension rheology in plane Couette flow and compared the viscous and frictional rheology frameworks. Our analysis of the simulations shows that the particle stress accounts for the largest part of the total shear stress. This particle stress consists of two parts of which the hydrodynamic part is larger for the low volume fractions while the contact part dominates for higher volume fractions. The volume fraction at which the contact part becomes larger than the hydrodynamic part decreases with increasing friction coefficient. We find that the relative viscosity, $\eta_r = \eta/\eta_0$, scales well with ϕ/ϕ_m , with ϕ_m obtained from fitting the Maron-Pierce correlation. For the friction rheology framework, we found that the macroscopic friction coefficient, μ , scales well with the viscous number, I_v . Furthermore, we find a monotonic relation between ϕ/ϕ_m and I_v , which depends only weakly on the Coulomb coefficient of sliding friction, μ_c . Since $\eta_r = \mu/I_v$, we thus find that the two frameworks are largely equivalent and that both account implicitly for Coulomb friction. However, we find that the normal particle stress differences, N_1 and N_2 , when normalized with the total shear stress and plotted against either ϕ/ϕ_m or I_v , remain explicitly dependent on μ_c in a manner that is not yet fully understood.

How does the suspension rheology under heterogeneous shear differ from the suspension rheology under homogeneous shear conditions?

In Chapter 4, we studied the suspension rheology in pressure-driven channel flow. First, we looked at the transient of the flow, focussing on the effect of solid volume fraction and friction coefficient on the particle migration timescale. The flow development time decays exponentially with increasing ϕ_b/Φ_R , where Φ_R is a friction-dependent reference bulk concentration beyond which particle contacts cause a rapid increase in the particle stress. Second, the steady-state rheology was studied by means of the ‘viscous’ and ‘frictional’ rheology frameworks. Excluding the central core and wall regions, the data for the local relative suspension viscosity collapse onto a single curve as a function of the normalized local concentration $\tilde{\phi}/\phi_m$, where ϕ_m is the friction-dependent maximum flowable packing fraction. The frictional rheology shows ‘subyielding’ at low viscous number I_v in the core region, where the macroscopic friction coefficient μ drops below the minimal value found for homogeneous shear flows. A modified frictional rheology model is presented that captures subyielding. Finally, a model is presented for $\tilde{\phi}/\phi_{mp}$ as a function of I_v , where ϕ_{mp} is a modified maximum flowable packing fraction. It captures both ‘overcompaction’ in the core beyond ϕ_m at high ϕ_b and maximum core concentrations below ϕ_m at lower ϕ_b .

Printability of dense suspensions in Liquid Deposition Modelling

The answers to the above research questions give more insight into the fundamental aspects of suspension rheology. However, PR-DNS simulations under these flow conditions are not feasible for day-to-day operations. In Chapter 5, we discussed how our results can be used to assess printability of dense suspensions. We identified the important rheological parameters for Liquid Deposition Modelling as the yield stress, the shear-thinning behavior, the viscoelasticity, the thixotropic time, and the stability. We estimated the yield stress from the DNS results in Chapter 4. This shows that the yield stress is a function of ϕ_b/ϕ_m and can be described by a Maron-Pierce [5] equation. Substituting this yield stress in the dimensionless number Ξ , introduced by M'Barki et al. [6], shows the printability of the suspension with $\Xi > 1$ for printable suspensions. The volume fraction where $\Xi = 1$ shifts depending on the printing conditions and the suspension properties, highlighting that this is a great tool to assess the printable region. Another tool used to assess printability are regime maps, which are typically based on the storage modulus and yield stress of a suspension. We are not able to make a regime map based on these properties, as we did not study the shear-rate dependent rheology. This is possible using our PR-DNS if the correct flow conditions are implemented, such as oscillatory shear. Furthermore, the extrusion pressure was analyzed in relation to the shear-thinning behavior of the suspension. A power-law model was fitted to the flow curves obtained for plane-channel flow in Chapter 4. This shows the dependence of the required extrusion pressure on the solid volume fraction and Coulomb coefficient of solid friction. The stability during printing was examined in terms of particle sedimentation in the supply tube of an idle printer. This shows that the sedimentation distance for typical suspensions is limited; however, Chapter 2 shows that heterogeneity and particle clusters develop at shorter timescales. Another factor in the stability is shear-induced particle migration, as observed in Chapter 4. We showed that, under typical printing conditions, complete migration can happen in tubes as short as 25cm. The results from Chapter 4 show that heterogeneity is already significant at much shorter lengths. The analysis of the results obtained in previous chapters in terms of the printability underlines that a good understanding of the parameters affecting the rheology of dense suspensions is key to develop both equipment and formulations for 3D-printing.

6.2 Recommendations

The questions we answered in this study are only a small part of the open questions on this topic. The rheology of dense suspensions is very complex and this work again shows that there are many factors that affect the rheology. In this section, we describe a number of recommendations to continue and expand on the results that we obtained.

To validate the results of our DNS study, experiments can be performed under similar flow conditions. The sedimentation can be experimentally studied using particle tracking, which has already been used for such experiments [7, 8, 9, 10] of settling particles at varying concentration and tube-to-particle diameter. The simulations on simple shear between parallel plates can be experimentally mimicked in a Taylor-Couette setup, or using a pressure-imposed shear cell [11]. Pressure-driven flow could be studied using for

example MRI, which gives insight into the particle velocities as well as the microstructure of the suspensions [12].

As discussed in Chapter 5, printability is strongly dependent on the shear-rate dependence of the rheology [13]. In this work we investigated the rheology at fixed shear rate to study the effect of solid volume fraction and friction coefficient. Extending the models we developed with a shear-rate dependence would be very useful for predicting printability. This expansion might be possible by combining existing models with our results; however, it is also possible to use our PR-DNS approach to study the effect of shear rate on the rheology of dense suspensions [14].

Another interesting aspect is the effect of polydispersity in particle size and shape. In reality, suspensions rarely have a monodisperse particle size, creating a need for models incorporating the effect of polydispersity. This topic has already received attention in the literature [15, 16], however, more work is needed to translate the suspension dynamics into constitutive rheological models. This topic is of interest specifically for 3D-printing of energetic materials as changing the particle size distribution and particle shape can act as a strategy to increase the maximum flowable packing fraction, and thus increasing the maximum printable solid volume fraction.

With respect to the timescale of particle migration in pressure-driven flow, it would be interesting to study the effect of Reynolds number on the migration behavior and its timescale. This is directly related to the migration in 3D-printing through the printing speed and the fluid phase viscosity of the suspension.

A related topic is the implementation of our modified frictional rheology model, established in Chapter 4, in the Suspension Balance Model. To compare SBM predictions with the DNS results, still a carefully validated constitutive model for the normal particle stress is required. Our DNS results indicate non-local suspension behavior in the channel core, where the wall-normal particle stress is correlated to the ‘rms shear’ viscous number (Θ_v) based on the square root of the granular temperature. Furthermore, outside the central core region, the rms shear viscous number appears fully correlated with the mean shear viscous number through a power-law relation. These findings support the suggestion of Nott and Brady [17] to base the constitutive relation for the wall-normal particle stress on the fluctuating shear rate, $\sqrt{T_g}/d$ where T_g is the granular (suspension) temperature, instead of the mean shear rate or, alternatively, as a function of both. This requires the extension of the SBM with an additional energy equation for the granular temperature. This approach has been shown already to overcome the problem of the classical SBM with the packing fraction at the channel centerline [17]. The SBM would be a useful tool to predict migration time and particle concentration distribution if the description of the rheology can indeed be improved.

As discussed in Chapter 1, we identified multiple stages in the printing process: (1) stationary suspension in the reservoir and tubes of the printer, (2) suspension flowing through the supply tube of the printer, (3) suspension flowing through the nozzle, and (4) suspension deposited on the printing platform. In this work we focussed on stages (1) and (2), that pertain to the flow behavior and rheology of dense suspensions. A logical next step would be to look at stage (3): suspension flowing through the nozzle. The effect of a contraction in a channel/tube should be studied, as it may have a large impact on the particle

distribution, as well as on the printability due to clogging of the nozzle [18, 19, 20]. Next to that, Chapter 5 shows that the suspension rheology is paramount to the shape retention in stage (4). This should also be taken into account in future work to be able to assess all aspects of the printability of suspensions.

References

- [1] Alfred W Francis. Wall effect in falling ball method for viscosity. *Physics*, 4(11):403–406, 1933.
- [2] JF Richarson and WN Zaki. Sedimentation and fluidisation: Part 1. *Trans. Ins. Chem. Eng*, 31:35–53, 1954.
- [3] Renzo Di Felice and Enrico Parodi. Wall effects on the sedimentation velocity of suspensions in viscous flow. *AIChE journal*, 42(4):927–931, 1996.
- [4] Xiaolong Yin and Donald L Koch. Hindered settling velocity and microstructure in suspensions of solid spheres with moderate reynolds numbers. *Physics of Fluids*, 19(9):093302, 2007.
- [5] Samuel H Maron and Percy E Pierce. Application of ree-yring generalized flow theory to suspensions of spherical particles. *Journal of colloid science*, 11(1):80–95, 1956.
- [6] Amin M’barki, Lydéric Bocquet, and Adam Stevenson. Linking rheology and printability for dense and strong ceramics by direct ink writing. *Scientific reports*, 7(1):6017, 2017.
- [7] S Heitkam, Y Yoshitake, F Toquet, D Langevin, and A Salonen. Speeding up of sedimentation under confinement. *Physical review letters*, 110(17):178302, 2013.
- [8] Hélène Nicolai and Elisabeth Guazzelli. Effect of the vessel size on the hydrodynamic diffusion of sedimenting spheres. *Physics of Fluids*, 7(1):3–5, 1995.
- [9] Laurence Bergougnoux and Élisabeth Guazzelli. Non-Poisson statistics of settling spheres. *Physics of Fluids*, 21(9), 2009.
- [10] Laurence Bergougnoux and Élisabeth Guazzelli. Dilute sedimenting suspensions of spheres at small inertia. *Journal of Fluid Mechanics*, 914:A33, 2021.
- [11] François Boyer, Élisabeth Guazzelli, and Olivier Pouliquen. Unifying suspension and granular rheology. *Physical review letters*, 107(18):188301, 2011.
- [12] Willian Hogendoorn, Wim-Paul Breugem, David Frank, Martin Bruschewski, Sven Grundmann, and Christian Poelma. From nearly homogeneous to core-peaking suspensions: Insight in suspension pipe flows using mri and dns. *Physical Review Fluids*, 8(12):124302, 2023.
- [13] Romain Mari, Ryohei Seto, Jeffrey F Morris, and Morton M Denn. Shear thickening, frictionless and frictional rheologies in non-brownian suspensions. *Journal of Rheology*, 58(6):1693–1724, 2014.
- [14] Elisabeth Lemaire, Frédéric Blanc, Cyrille Claudet, Stany Gallier, Laurent Lobry, and François Peters. Rheology of non-brownian suspensions: a rough contact story. *Rheologica Acta*, 62(5):253–268, 2023.

- [15] Sidhant Pednekar, Jaehun Chun, and Jeffrey F Morris. Bidisperse and polydisperse suspension rheology at large solid fraction. *Journal of Rheology*, 62(2):513–526, 2018.
- [16] Nathan J Di Vaira, Łukasz Łaniewski-WoŃk, Raymond L Johnson, Saïed M Aminossadati, and Christopher R Leonardi. Influence of particle polydispersity on bulk migration and size segregation in channel flows. *Journal of Fluid Mechanics*, 939:A30, 2022.
- [17] Prabhu R Nott and John F Brady. Pressure-driven flow of suspensions: simulation and theory. *Journal of Fluid Mechanics*, 275:157–199, 1994.
- [18] Alvaro Marin, Henri Lhuissier, Massimiliano Rossi, and Christian J Kähler. Clogging in constricted suspension flows. *Physical Review E*, 97(2):021102, 2018.
- [19] Mathieu Souzy, Iker Zuriguel, and Alvaro Marin. Transition from clogging to continuous flow in constricted particle suspensions. *Physical Review E*, 101(6):060901, 2020.
- [20] Alvaro Marin and Mathieu Souzy. Clogging of noncohesive suspension flows. *Annual Review of Fluid Mechanics*, 57, 2024.

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Scientific Contributions

Journal publications

1. **Wouter Peerbooms**, Antoine van der Heijden, Wim-Paul Breugem; Viscous sedimentation of dense suspensions in narrow vertical tubes. Manuscript in preparation
2. **Peerbooms, W.**, Heijden, A.v.d. & Breugem, W.P. Transient behavior and steady-state rheology of dense frictional suspensions in pressure-driven channel flow. *Acta Mech* 236, 5681–5714 (2025). <https://doi.org/10.1007/s00707-024-04106-7>
3. **Wouter Peerbooms**, Tim Nadorp, Antoine van der Heijden, Wim-Paul Breugem; Interparticle friction in sheared dense suspensions: Comparison of the viscous and frictional rheology descriptions. *J. Rheol.* 1 March 2024; 68 (2): 263–283. <https://doi.org/10.1122/8.0000729>

Conference contributions

1. Oral presentation at Burgers Symposium 2023, Lunteren, The Netherlands: Influence of solid friction on the rheology of dense suspensions in plane Couette flow; **W. Peerbooms**, T. Nadorp, A.E.D.M. van der Heijden, W.P. Breugem
2. Oral presentation at the 14th European Fluid Mechanics Conference 2022, Athens, Greece: Rheology of dense suspensions in pressure-driven channel flow: influence of solid friction; **W. Peerbooms**, A.E.D.M. van der Heijden, W.P. Breugem
3. Oral presentation at Burgers Symposium 2022, Lunteren, The Netherlands: Influence of solid friction on the rheology of dense suspensions in pressure-driven channel flow; **W. Peerbooms**, A.E.D.M. van der Heijden, W.P. Breugem
4. Poster presentation at Physics at Veldhoven 2022, Online: Sedimentation of dense suspensions in narrow tubes; **Wouter Peerbooms**, Antoine van der Heijden, Wim-Paul Breugem
5. Oral presentation at IECCEM 2021, Online: Sedimentation of Dense Suspensions in Narrow Tubes; **Wouter Peerbooms**, Antoine van der Heijden, Wim-Paul Breugem
6. Project pitch at TNO PhD conference 2021, Eindhoven, The Netherlands

Datasets

1. **Peerbooms, Wouter**; van der Heijden, Antoine E. D. M.; Breugem, Wim-Paul (2026): Data corresponding to the research: "Viscous sedimentation of dense suspensions in narrow vertical tubes". Version 1. 4TU.ResearchData. dataset. <https://doi.org/10.4121/21564105>
2. **Peerbooms, Wouter**; van der Heijden, Antoine E. D. M.; Breugem, Wim-Paul (2024): Data corresponding to the publication: "Transient behavior and steady-state rheology of dense frictional suspensions in pressure-driven channel flow". Version 1. 4TU.ResearchData. dataset. <https://doi.org/10.4121/e7c86771-72bb-48da-b9f9-6c0857655404.v1>

3. **Peerbooms, Wouter**; Nadorp, Tim; van der Heijden, Antoine E. D. M.; Breugem, Wim-Paul (2024): Data corresponding to the publication: "Interparticle friction in sheared dense suspensions: Comparison of the viscous and frictional rheology descriptions". Version 1. 4TU.ResearchData. dataset. <https://doi.org/10.4121/bbb1d553-7230-4a60-80a2-23d5697d89a5.v1>