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Understanding the effects of particle properties and particle-scale flow on suspension rheology

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Abstract

Dense suspensions of solid particles immersed in a liquid are ubiquitous in industries. Understanding the rheology of dense suspensions plays an important role in improving industrial processes. In this thesis, the coupling of the Lattice Boltzmann Method (LBM), a class of computational fluid dynamics (CFD) methods for fluid simulation, and the Discrete Element Method (DEM), an effective numerical method in the analysis of granular systems, have been employed to simulate the non-Brownian dense suspensions. Such LBDEM simulations can capture the detailed flow field in the particle level and reveal the effect of the interactions between background fluid and particles.

We conduct DEM simulations of a binary model system composed of frictional and frictionless particles (Chapter 4) and investigate the relationship between the jamming volume fraction of dense suspension and the fraction f of frictional contacts, which is determined by the fraction of frictional particles. By comparing our data with simulations of shear thickening suspensions, which introduce a transition between frictional and frictionless contacts by the Critical Load Model (CLM), we show that the Wyart-Cates model of shear thickening is incomplete. The shear-thickening behaviour is then successfully captured by LBDEM simulations of dense suspensions under simple shear (Chapter 5). The difference between LBDEM and DEM simulations of suspensions can be minor in terms of the bulk rheology because the averaged velocity fields under simple shear are similar for these two simulation approaches. The third part is the LBDEM simulations of pressure-driven flow in the square channel (Chapter 6), where interactions between fluid and particles are not negligible and cannot be captured by DEM simulations. We capture the shear-induced migration of suspensions in the channel and look into the effect of friction in the migration process. With detailed information of the fluid phase from LBM and the solid phase from DEM, we examine the suspension balance model for different volume

fractions and friction coefficients. These results can serve as a database for the further theoretical study of pressure-driven flow.

Lay Summary

Suspensions, mixtures of solid particles and liquid, are common in nature and industry. From cement and ceramic pastes to 3D printing, paints and drilling fluids, the engineering challenges associated with suspensions have been studied for decades, yet a thorough knowledge of dense suspension flows is still lacking. The understanding and prediction on suspension flow can contribute to optimizing industrial manufacturing. The first part of this thesis is about particle-based simulations of a binary model system consisting of two species of particles disparate in surface friction, which helps us understand more about the role of friction in suspension viscosity under simple shear flow. We also conduct a series of fluid-solid coupling simulations, which captures the motion of solid particles and resolves the detailed fluid flow around the particles in two different well-defined conditions: simple shear flow and channel flow. These simulations successfully capture the shear thickening behaviour under simple shear as well as the shear-induced particle migration in the channel, and reveal the effect of the interaction between background fluid and particles. Our results contribute to the further completion of the continuum two-phase model, which assumes the interstitial fluid and the particles are two intertwined continuous phases, and prediction on the suspension flow behaviour.

Declaration

I declare that this thesis was composed by myself, that the work contained herein is my own except where explicitly stated otherwise in the text, and that this work has not been submitted for any other degree or professional qualification except as specified.

(Yang Cui, Nov 2022)

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Chapter 1

Introduction

Mixtures of a fluid and particles, described as suspensions, are ubiquitous in nature and industry, for example, mud, pharmaceuticals and 3D-printing. The physics of suspensions flows are however complex, especially at high volume fractions, where the flow behavior becomes increasingly unstable and unpredictable. With the rapid development of parallel computing, simulations has become a helpful tool in addition to experiments. Various methods have been proposed to simulate fluid-particle flows. However, most simulation works, based on a constitutive description of fluid phase or solid phase, ignored the local fluid field at particle level, which resulted in the lack of convincing description for complex background fluid and specific geometries. Recently, the coupling of Lattice Boltzmann Method (LBM), a class of computational fluid dynamics (CFD) methods for fluid simulation, and Discrete Element Method (DEM), an effective numerical method in the analysis of granular systems, have been employed to simulate the suspension systems, which captures the detailed flow field in particle level. The effect of the interaction between background fluid and particles can be revealed by such simulation works.

1.1 Thesis outline

We begin the thesis by introducing the requisite background in rheology in Chapter2: including the formal framework of rheology and rheology of suspensions. Two typical rheological phenomena are discussed here, including

shear-thickening behaviour, induced by the inter-particle interactions, and shear-induced migration, induced by the relative motion between fluid and solid particles.

The simulation methods are then reviewed in Chapter 3: including the discrete element method (DEM) for the solid phase and the lattice Boltzmann method (LBM) for the fluid phase. Some popular approaches for the coupling between DEM and LBM are discussed, and a whole procedure of LBM-DEM coupling is summarized in the end.

Our results are divided into three parts. Chapter 4 reports DEM simulations of a binary model system composed of frictional and frictionless particles. We first investigate the relationship between the jamming volume fraction of dense suspension and the fraction of frictional particles, which determines the fraction f of frictional contacts. The comparison between our results and the Wyart-Cates model, which captures the shear thickening behaviour of dense suspensions, indicates that a single scalar parameter f is inadequate to predict the rheology of such a binary system.

Simulations of sheared suspensions are conducted with the coupled lattice Boltzmann discrete element method (LBDEM). The viscosity divergences for frictional and frictionless particles and the shear-thickening behaviour of dense suspensions are successfully captured. In this chapter (Chapter 5), our simulation results are fitted by two constitutive models proposed by Krieger and Dougherty [62] and Boyer et al. [11] and related critical values like jamming volume fraction, and critical macroscopic friction coefficient are captured for our simulation system. Moreover, the difference between LBDEM and DEM simulations is found to be minor in terms of the bulk rheology of dense suspensions under simple shear.

Chapter 6 focuses on the LBDEM simulations of pressure-driven flow in the square channel, where the relative motion between fluid and particles is not negligible and cannot be captured by DEM simulations. The shear-induced migration of suspensions in the channel and the over-compaction, where the volume fraction is higher than the jamming limit ϕ_m , at the centre of the channel are successfully captured. The suspension balance model, proposed by Morris and Boulay [92], are examined with detailed information on the fluid phase and the solid phase. Particle-level information in the over-compaction region is also presented and can serve as a solid database for the further theoretical modelling of dense suspensions under inhomogeneous flow.

The thesis finishes with a summary and conclusion chapter(Chapter 7), followed by recommendations for possible future work.

Chapter 2

Background

Rheology, coined by Eugene C. Bingham, a professor at Lafayette College, in 1920 and originated from the Greek phrase study of flow is the science that deals with the flow and deformation behaviour of materials, both solids and liquids, when subjected to forces or stresses.

As a fundamental part of material science, rheology is principally concerned with applying elasticity and fluid mechanics to characterise the flow of materials which exhibits elastic, viscous and plastic behaviour when subjected to stress. It is also concerned with explaining and predicting mechanical behaviour based on the microstructure of materials. Rheology has been introduced to many fields, including non-equilibrium physics, geoscience, biology and pharmaceuticals. Rheology also has numerous applications in industrial processes, e.g. cement, paint, plastics, drilling muds and food products. Therefore, understanding the rheology of materials and applying the rheology to optimise industrial manufacturing is of vital importance.

In this chapter, we first outline the basic framework of continuum mechanics and introduce a simple case - Newtonian fluids under the simple shear. We then narrow the topic to suspension rheology and start with the bulk rheological properties of dense suspensions under simple shear. Finally, we extend the discussion to non-Newtonian (shear-thickening) behaviours and inhomogeneities in complex geometries (channel flow and extrusion), respectively.

2.1 Principles of rheology

2.1.1 General deformations

Strain and strain rate tensor In continuum mechanics, the material is treated as a set of small elements to characterise deformation¹. The idea is also applied in the research of rheology. As shown in Figure 2.1, the state of deformation at a small cubic element P can be characterised by the infinitesimal strain tensor $E_{\alpha\beta}$ ²:

$$E_{\alpha\beta} = \frac{1}{2} \left(\frac{\partial X_\alpha}{\partial x_\beta} + \frac{\partial X_\beta}{\partial x_\alpha} \right) \quad (2.1)$$

where $\mathbf{x}$ and $\mathbf{X}(\mathbf{x}, t)$ are, respectively, the position and displacement of element P to the reference state. Analogously, the strain-rate tensor $\dot{\Gamma}_{\alpha\beta}$ can be expressed as:

$$\dot{\Gamma}_{\alpha\beta} = \frac{1}{2} \left(\frac{\partial v_\alpha}{\partial x_\beta} + \frac{\partial v_\beta}{\partial x_\alpha} \right) \quad (2.2)$$

where $\mathbf{v}(\mathbf{x}, t) = \dot{\mathbf{X}}(\mathbf{x}, t)$ is the local velocity field. In both strain and strain-rate tensors, the diagonal terms ($\alpha = \beta$) and the off-diagonal terms ($\alpha \neq \beta$) refer to the elongation in α direction and shearing deformations in $\alpha - \beta$ plane, respectively.

Stress tensor In continuum mechanics, strain measures the deformation of the material, while stress expresses the internal forces which are generated from the relative motion of neighbouring elements. Stress acting on the surface of the cubic element P has units of force/area, i.e. Pa in SI units, and is characterised by a stress tensor $\boldsymbol{\sigma}$, which is depicted in Figure 2.1 (B) and can be written as:

$$\boldsymbol{\sigma} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix} \quad (2.3)$$

Here $\sigma_{\alpha\beta}$ denotes the force per unit area in the β direction acting on the plane with normal vector in α direction. Similar to strain and strain rate tensors, the diagonal terms ($\alpha = \beta$), i.e. σ_{xx} , σ_{yy} , σ_{zz} , and the off-diagonal terms ($\alpha \neq \beta$),

¹Analysis in this section is mainly taken from lecture courses (Continuum Mechanics and Granular Matter) given by Professor Yujie Wang and Professor Jie Zhang in the Department of Physics at Shanghai Jiao Tong University between 2014 and 2016.

²Here α, β refer to spatial directions x, y, z

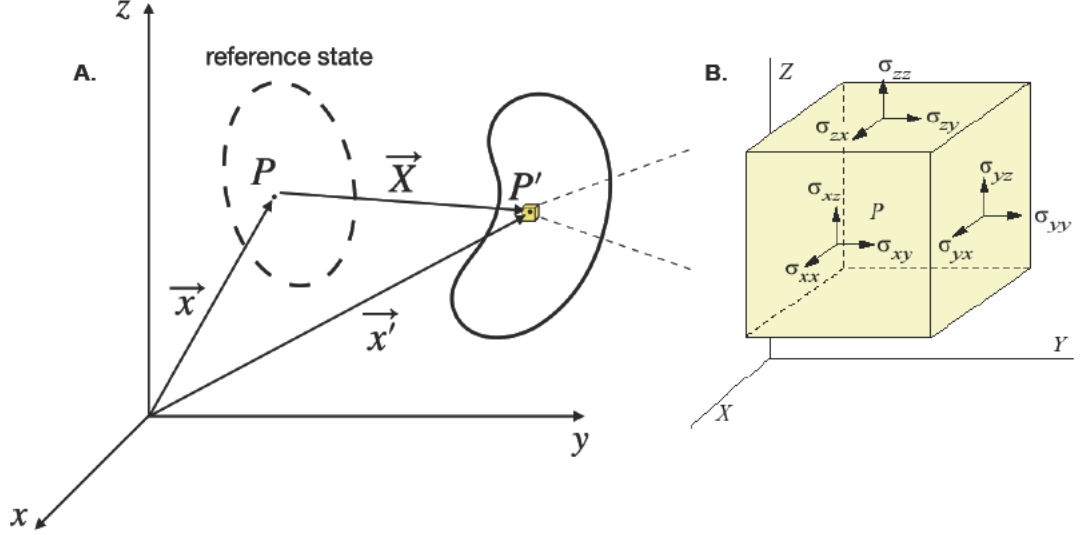


Figure 2.1 A. Sketch of a general deformation in continuum mechanics. B. Nine components of stress in three dimensions, taken from Jiang [53]

e.g. σ_{xy} represent the normal stresses and shear stresses, respectively. The stress tensor is symmetric ($\sigma_{\alpha\beta} = \sigma_{\beta\alpha}$) for most materials, including the suspensions discussed in this thesis. More discussions can be found in Macosko [85].

The stress tensor $\sigma_{\alpha\beta}$ can be expressed as the sum of two other stress tensors.

$$\begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix} = \begin{pmatrix} p & 0 & 0 \\ 0 & p & 0 \\ 0 & 0 & p \end{pmatrix} + \begin{pmatrix} \sigma'_{xx} & \sigma'_{xy} & \sigma'_{xz} \\ \sigma'_{yx} & \sigma'_{yy} & \sigma'_{yz} \\ \sigma'_{zx} & \sigma'_{zy} & \sigma'_{zz} \end{pmatrix} \quad (2.4)$$

The first term in the right side of Equation 2.4 is the mean normal tensor, $-p\delta_{\alpha\beta}$, which tends to change the volume of the element P . The second term is called the deviatoric stress tensor, denoted by $\tau_{\alpha\beta}$, which tends to distort the element P . Thus, the above equation can be written as:

$$\sigma_{\alpha\beta} = -p\delta_{\alpha\beta} + \tau_{\alpha\beta} \quad (2.5)$$

where $\delta_{\alpha\beta}$ is the Kronecker delta and $p = -\frac{1}{3}\sigma_{\alpha\alpha} = -\frac{1}{3}(\sigma_{xx} + \sigma_{yy} + \sigma_{zz})$ is the mechanical pressure. The deviatoric stress tensor is traceless, i.e. $\sigma'_{xx} + \sigma'_{yy} + \sigma'_{zz} = 0$. The stress tensor and deformation tensors, including strain tensor and strain rate tensor, are related by a constitutive function:

$$\boldsymbol{\sigma} = \mathcal{F}(\mathbf{E}, \dot{\mathbf{\Gamma}}) \quad (2.6)$$

where $\boldsymbol{\sigma}$ denotes the stress tensor $\sigma_{\alpha\beta}$. In general, the constitutive function $\mathcal{F}$ requires too many components to construct the relationship between three second-rank tensors in three dimension space. Here we first introduce a simple case - Newtonian fluid under simple shear for illustration.

2.1.2 Newtonian fluid

The motion of a continuous fluid can be described by the Navier-Stokes equations: the equation for conservation of momentum:

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = \nabla \cdot \boldsymbol{\sigma} + \mathbf{f} \quad (2.7)$$

and the continuity equation for incompressible fluid:

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

where ρ is the density of the fluid, $\mathbf{u}$ is the velocity vector, $\boldsymbol{\sigma}$ is the stress tensor, $\mathbf{f}$ is the external force per unit volume acting on the fluid, and ∇ is the gradient operator.

In the steady Stokes flow, a type of fluid flow where inertial forces are negligible compared to viscous forces³, the temporal change, described by $\rho \frac{\partial \mathbf{u}}{\partial t}$, and the convection acceleration, described by $\mathbf{u} \cdot \nabla \mathbf{u}$, of the fluid flow can be neglected⁴.

For a Newtonian fluid, in which the stress tensor and strain-rate tensor are linearly related, the stress tensor can be written as:

$$\boldsymbol{\sigma} = -p\mathbf{I} + 2\eta\dot{\boldsymbol{\Gamma}} \quad (2.9)$$

where $\mathbf{I}$ is the unit tensor. η is the viscosity of the Newtonian fluid and has a unit of Pa·s in SI units.

Therefore, in steady Stokes flow of a Newtonian fluid, the Navier-Stokes equation can be written as:

$$\eta \nabla^2 \mathbf{u} - \nabla p + \mathbf{f} = 0 \quad (2.10)$$

³The ratio between inertial force and viscous force are measured by Reynolds number and Stokes number, corresponding mathematical expressions can be found in Section 2.2.1

⁴Details can be found in [36]

Simple shear Here we illustrate a simple shear, which provides the simplest form of strain rate tensor $\dot{\mathbf{\Gamma}}$ for a further simplification of the constitutive function mentioned above. As shown in Figure 2.2, incompressible, isotropic fluid is contained between infinite parallel plates with separation H , and the upper plate moves with a constant velocity $\mathbf{U} = (U, 0, 0)$. Given the laminar flow and the non-slip boundary condition, i.e. no relative motion between the upper plate and the fluid layer close to the upper plate, the fluid velocity field $(u_x(y), 0, 0)$ has only one non-zero component parallel to $\mathbf{U}$, and the gradient of fluid velocity field $u_x(y)$ is constant and perpendicular to the velocity itself:

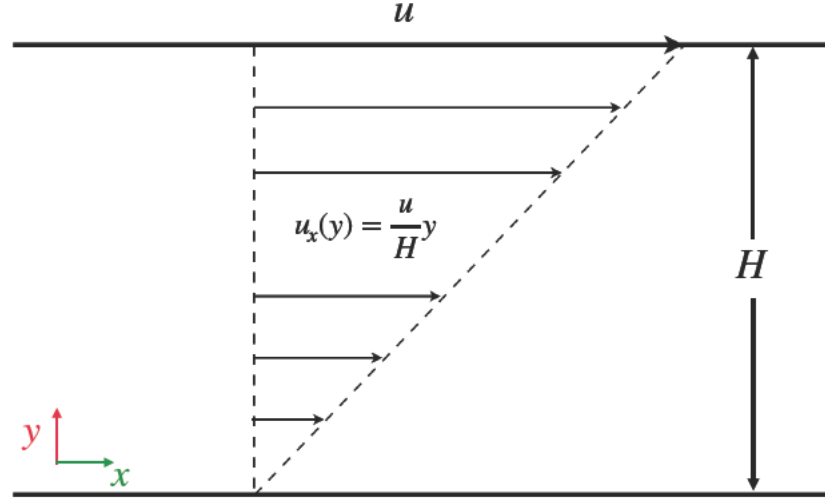


Figure 2.2 Sketch of a simple shear in a 2D plane. The upper plate moves with velocity $\mathbf{u} = (u, 0, 0)$ in Cartesian coordinates.

$$\frac{\partial u_x}{\partial y} = \frac{U}{H} = \dot{\gamma} \quad (2.11)$$

where $\dot{\gamma}$ is the shear rate and $\frac{\partial u_x}{\partial x} = \frac{\partial u_x}{\partial z} = 0$. Thus the strain-rate tensor for simple shear flow has only one non-zero term and can be written as:

$$\dot{\mathbf{\Gamma}} = \begin{bmatrix} 0 & \dot{\gamma} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad (2.12)$$

Simple shear with the rate $\dot{\gamma}$ is the combination of pure shear strain with the rate of $\frac{1}{2}\dot{\gamma}$ and rotation with the rate of $\frac{1}{2}\dot{\gamma}$:

$$\dot{\mathbf{\Gamma}} = \underbrace{\begin{bmatrix} 0 & \dot{\gamma} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}}_{\text{simple shear}} = \underbrace{\begin{bmatrix} 0 & \frac{1}{2}\dot{\gamma} & 0 \\ \frac{1}{2}\dot{\gamma} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}}_{\text{pure shear}} + \underbrace{\begin{bmatrix} 0 & \frac{1}{2}\dot{\gamma} & 0 \\ -\frac{1}{2}\dot{\gamma} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}}_{\text{rotation}} \quad (2.13)$$

Here the rotation part has no contribution to the deformation of materials. Thus we can combine Equation 2.9 and the pure shear described above to get the well-known constitutive relation for Newtonian fluids under simple shear, which is:

$$\sigma_{xy} = \eta \dot{\gamma} \quad (2.14)$$

Similarly, the constitutive relation for Hookean solids under simple shear can be written as:

$$\sigma_{xy} = G\gamma \quad (2.15)$$

where γ is the shear strain and G is the shear modulus.

2.1.3 Non-Newtonian fluid

Although Newtonian fluids are the simplest mathematical models of fluids that account for viscosity and are quite common in our daily life, such as water and honey at room temperature, non-Newtonian fluids, in which the viscosity is dependent on stress, are also ubiquitous such as cornstarch suspensions, toothpaste, blood and shampoo.

Normal stress differences For non-Newtonian fluids, Equation (2.9) no longer holds and the stress tensor $\boldsymbol{\sigma}$ under simple shear has the form:

$$\boldsymbol{\sigma} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & 0 \\ \sigma_{yx} & \sigma_{yy} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix} \quad (2.16)$$

Here the x, y, z directions are the flow, gradient and vorticity directions. If the fluid is incompressible, the pressure, i.e. the trace of the stress tensor is of no rheological interest as it is prescribed by the flow and the two related quantities

are the first N_1 and second N_2 normal-stress differences:

$$N_1 = \sigma_{xx} - \sigma_{yy} \quad \text{and} \quad N_2 = \sigma_{yy} - \sigma_{zz} \quad (2.17)$$

The normal stress difference is related to the degree of anisotropy in the fluid, and it plays an important role in determining the behavior of the fluid. In some non-Newtonian fluids, such as shear-thickening fluids, the normal stress difference can be very large and can lead to complex patterns of deformation and mixing.

In suspension systems, the normal stress is related to the particle concentration and the particle size distribution. The normal stress can lead to particle migration and segregation, which can have important implications for industrial processes such as filtration and sedimentation⁵.

Types of non-Newtonian fluid In non-Newtonian fluids, it is usually assumed that these stresses depend only on the local value of the shear rate $\dot{\gamma}$: $\sigma_{xy} = \sigma_{xy}(\dot{\gamma})$, $N_1 = N_1(\dot{\gamma})$ and $N_2 = N_2(\dot{\gamma})$. Here we just briefly discuss some typical types of non-Newtonian fluids, based on the relation between shear stress (σ_{xy} , note as σ in Figure 2.3) and viscosity (η).

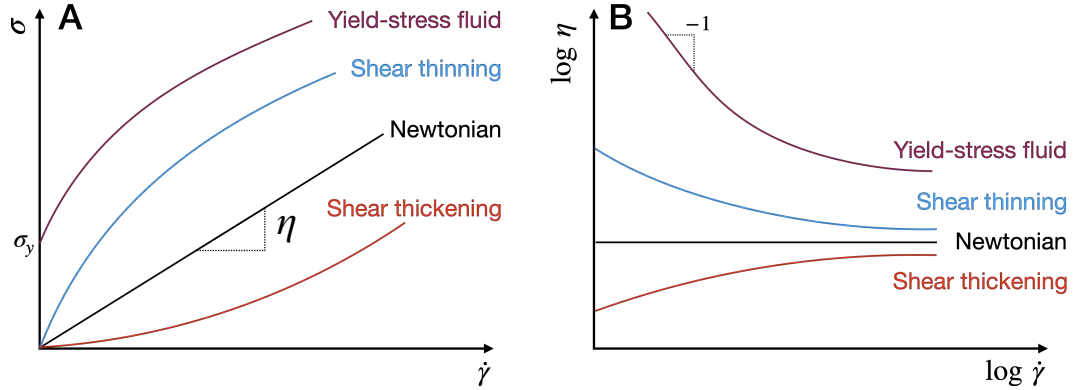


Figure 2.3 Schematic flow curves of Newtonian behaviour and some typical non-Newtonian behaviours of materials, including yield-stress, shear thinning and shear thickening fluid. (A): shear stress vs shear rate ($\sigma - \dot{\gamma}$). (B) log-log plot of viscosity vs shear rate ($\eta - \dot{\gamma}$)

If viscosity η decreases with shear rate $\dot{\gamma}$ (Figure 2.3B, blue curve), i.e. σ_{xy}

⁵The above two paragraphs are generated by ChatGPT. The prompt words include suspension, non-Newtonian and normal stress differences.

increases sublinearly with $\dot{\gamma}$ (Figure 2.3A, blue curve), the fluid is said to be shear thinning. Some common examples of shear-thinning fluids are ketchup, paints and blood. If viscosity η increases with shear rate $\dot{\gamma}$ (Figure 2.3B, red curve), i.e. σ_{xy} increases superlinearly with $\dot{\gamma}$ (Figure 2.3A, red curve), the fluid is said to be shear thickening. A typical example of a shear-thickening fluid is a mixture of cornstarch and water. For yield-stress fluid, indicated by the purple curve in Figure 2.3, the fluid stays static until the shear stress exceeds a critical stress value σ_y . The toothpaste we use every day is a typical kind of yield stress fluid.

2.2 Rheology of suspensions

Suspensions, refer to mixtures composed of solid particles immersed in a liquid, are ubiquitous in our daily life and industrial processes. Such systems have intrigued many researchers for decades but still remain a great challenge, especially for their rheology. Here we mainly talk about the rheology of non-Brownian, rigid and neutrally buoyant particles suspended in a Newtonian fluid.

For properly capturing the rheology of a simple sheared suspension mentioned here, some non-dimensionless numbers have to be introduced before the focus is shifted to the constitutive model.

2.2.1 Dimensional analysis of suspension systems

Here we consider a suspension system that consists of an incompressible Newtonian fluid of density ρ_f and dynamic viscosity η_f with monodisperse, rigid, neutrally buoyant solid particles with density $\rho_p = \rho_f$, diameter d , friction coefficient μ_p and elastic stiffness k_n . The whole suspension is imposed to a simple shear with a constant shear rate $\dot{\gamma}$, and the corresponding shear stress is σ . Thus, some dimensionless numbers are listed below.

Relative viscosity:

$$\eta_r = \eta_{suspension} / \eta_f = \frac{\sigma}{\dot{\gamma} \eta_f} \quad (2.18)$$

Solid volume fraction, or particle volume fraction:

$$\phi_s = \frac{V_p}{V} = \frac{1}{6}\pi d^3 \frac{N}{V} \quad (2.19)$$

where N and d are, respectively, the number and diameter of solid particles. And V and V_p are, respectively, the volume occupied by the whole suspension and solid particles.

The Stokes number and Reynolds number are defined as the ratio between fluid inertial forces and viscous forces for measuring the importance of inertia:

$$\text{St} = \frac{\rho_p \dot{\gamma} d^2}{\eta_f} \quad (2.20)$$

$$\text{Re}_p = \frac{\rho_f \dot{\gamma} d^2}{\eta_f} = \frac{\rho_f}{\rho_p} \text{St} \quad (2.21)$$

For neutrally buoyant suspended particles, i.e. $\rho_f = \rho_p = \rho$, the Stokes number and Reynolds number are identical.

The Peclet number is the ratio between time scales of imposed shear and Brownian diffusion for classifying between Brownian and non-Brownian regimes:

$$\text{Pe} = \frac{\tau_B}{1/\dot{\gamma}} = \frac{3\pi\eta_f \dot{\gamma} d^3}{4k_B T} \quad (2.22)$$

where k_B is the Boltzmann constant and T is the temperature. Stickel and Powell [124] show that the rheological behaviour can be classified into Newtonian, shear-thinning, and shear-thickening regimes based on the combination of the Reynolds number and Peclet number.

In the dry-granular case, the inertial number describes the ratio of inertial time of particle rearrangement on microscale to time of strain (macroscale) is proposed by MIDI [88] and Jop et al. [55]:

$$I = d \sqrt{\rho_p / P^p \dot{\gamma}} \quad (2.23)$$

where P^p is the confining pressure. Following that, Boyer et al. [11] introduced the viscous number in suspension systems:

$$I_v = \frac{\eta_f \dot{\gamma}}{P^p} \quad (2.24)$$

Here the viscous number can also be interpreted as the ratio of the typical viscous stress, $\eta_f \dot{\gamma}$, to the confining pressure, P^p , of the suspension system. [37].

2.2.2 Theoretical development

Adding solid particles into a Newtonian fluid increases the relative viscosity η_r and makes the whole suspension more complex and unpredictable. The time arrow in Figure 2.4 coincides with the evolution of research progress towards the understanding of more concentrated suspensions[37]. The relative viscosity of suspensions described above can be expressed by the constitutive equation $\eta_r = \eta/\eta_f = \frac{\sigma}{\dot{\gamma}\eta_f} = f(\phi)$, a volume fraction dependent equation.

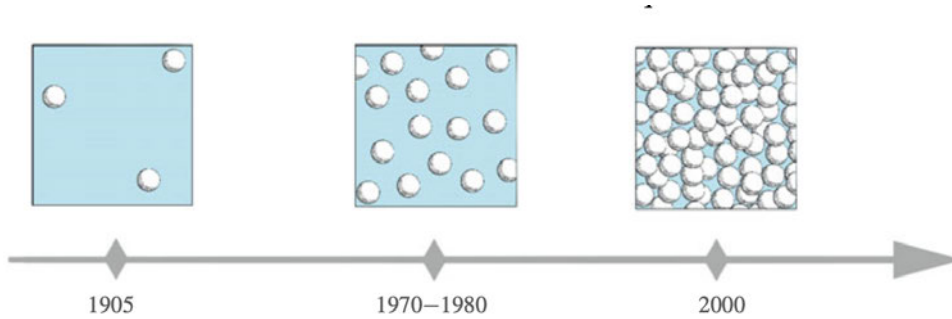


Figure 2.4 History of understanding of suspension rheology. Dilute suspensions in 1905, semi-dilute suspensions between 1970 and 1980 and dense suspensions from 2000. Figure is taken from Guazzelli and Pouliquen [37]

Dilute suspensions For very dilute suspensions, i.e. up to $\phi_s \approx 0.05$ [37] where particle-particle interaction through the ambient fluid is negligible. Einstein gave the expression in 1905 and the modification in 1911.

Einstein(1905) [27]:

$$\eta_r = 1 + \phi \quad (2.25)$$

Einstein(1911) [28]:

$$\eta_r = 1 + 2.5\phi \quad (2.26)$$

Semi-dilute suspensions Batchelor and Green [5] took particle-particle interactions into consideration and extended the previous relationship, i.e. up to

$\phi_s \approx 0.1 - 0.15$, to a second order approximation:

$$\eta_r = 1 + 2.5\phi + 7.6\phi^2 \quad (2.27)$$

Dense suspensions For higher solid fractions, multi-body interactions become dominant, and a first-principle model is still lacking. Different kinds of phenomenological equations have been proposed to correlate the viscosity of concentrated suspensions to the solid volume fraction. One of the most popular relationships is proposed by Krieger and Dougherty [62]. The Krieger and Dougherty relationship reads as follows:

$$\eta_r = \eta_0 \left(1 - \frac{\phi}{\phi_c}\right)^{-\alpha} \quad (2.28)$$

where ϕ_c is the critical volume fraction that represents where the viscosity diverges, i.e. at which the system transitions from liquid-like to solid-like. And the critical value ϕ_c is dependent on the friction coefficient of solid particles. As shown in Figure 2.5 taken from Guazzelli and Pouliquen [37], there are clearly two ϕ dependent curves which diverge at $\phi_c^{\mu_p \neq 0} \approx 0.60$ and at $\phi_c^{\mu_p = 0} \approx 0.64$ for frictional and frictionless particles. Here $\phi_c^{\mu_p = 0} \approx 0.64$ is the random close packing fraction and $\phi_c^{\mu_p \neq 0} \approx 0.60$ is the random loose packing fraction for $\mu = 0.5$. The Einstein viscosity is recovered when exponent index $\alpha = 2.5$, while $\alpha = 2$ gives better fitting results for high volume fractions.

Detailed description for Figure 2.5. Experiments: of Boyer et al. [11] using pressure-imposed rheometry with polystyrene (PS) spheres of diameter $d = 580\mu\text{m}$ suspended in polyethylene glycol-ran-propylene glycol monobutyl ether as well as poly(methyl methacrylate) (PMMA) spheres of diameter $d = 1100\mu\text{m}$ suspended in a Triton X – 100 /water/zinc chloride mixture; of Bonnoit et al. [9] using an inclined plane rheometer tilted at two different angles with PS spheres of diameter $d = 40\mu\text{m}$ suspended in silicone oil; of Dagois-Bohy et al. [22] using pressure-imposed rheometry with PS spheres of diameter $d = 580\mu\text{m}$ suspended in polyethylene glycol-ran-propylene glycol monobutyl ether; of Dbouk et al. [23] using a parallel-plate rotational rheometer with PS spheres of diameter $d = 140\mu\text{m}$ suspended in a mixture of water, UCON oil and zinc bromide; of Ovarlez et al. [103] using MRI technique and a wide-gap Couette geometry with PS spheres of diameter $d = 290\mu\text{m}$ suspended in silicone oil; and of Zarraga et al.

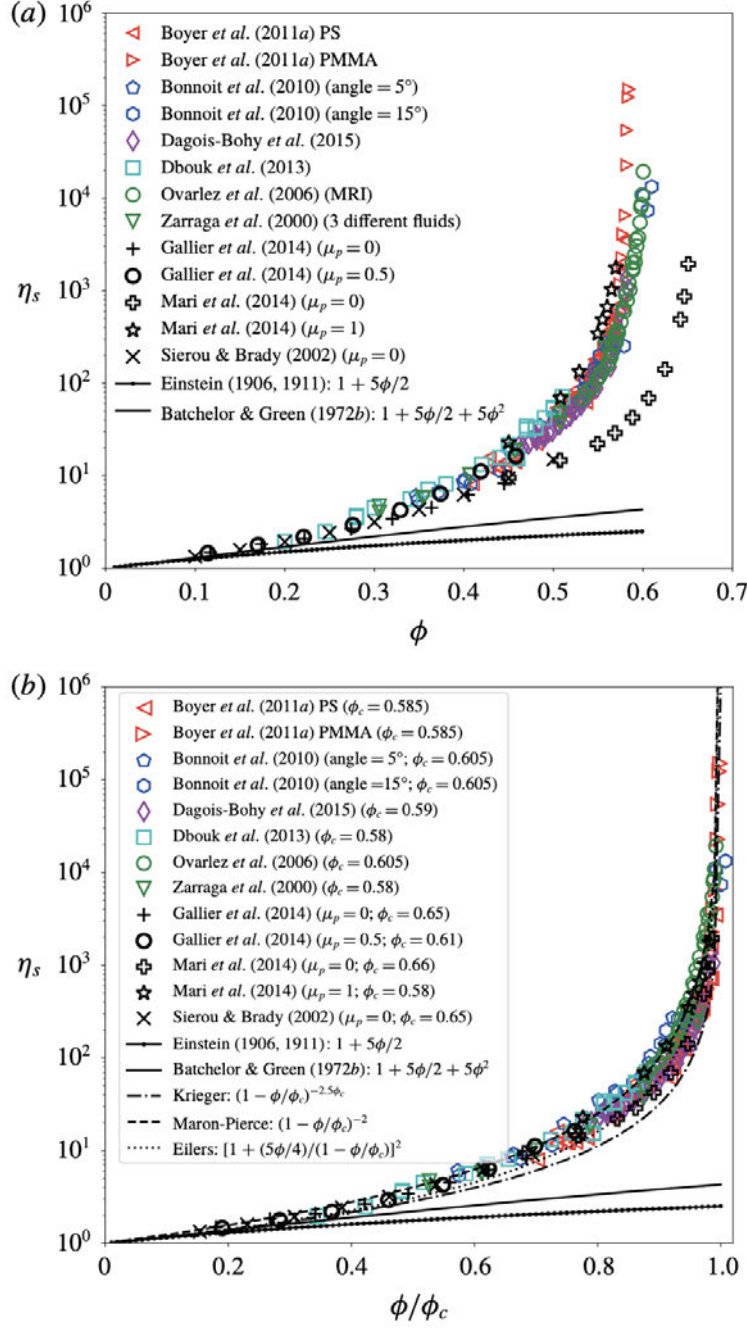


Figure 2.5 Relative viscosity, η_s , versus (a) volume fraction, ϕ , and (b) reduced volume fraction, ϕ/ϕ_c . Results are taken from different experiments, simulations and theoretical predictions. This figure and corresponding explanation are taken from Guazzelli and Pouliquen [37].

[138] using a parallel-plate rotational rheometer with glass spheres of diameter $d = 44\mu\text{m}$ suspended in three different fluids. Numerical simulations: of Sierou and Brady [117] and Gallier et al. [30] with ($\mu_p = 0.5$) and without ($\mu_p = 0$) friction; as well as those of Mari et al. [86] Mari et al. (2014) with ($\mu_p = 1$) and without ($\mu_p = 0$) friction, where μ_p is the friction coefficient between the spheres. Viscosity laws: of Einstein [27] and Einstein [28], of Batchelor and Green [5], of Krieger with exponent $\alpha = -2.5\phi_c$ and $\alpha = -2$ (Maron-Pierce), and of Eilers Stickel and Powell [124]. The corresponding ϕ_c used for each set of data in panel (b) are indicated in the legend.

2.2.3 Shear thickening

The discussion above is restricted to the Newtonian behaviour of suspensions, i.e. the viscosity of suspension η_r is independent of shear rate $\dot{\gamma}$. Whereas shear thickening behaviour is also widely observed in dense suspensions [133][18][39]. A typical example is a suspension of cornstarch particles, which acts like a solid at high shear rate and a liquid at low shear rate. Many interesting and counterintuitive videos about the shear thickening behaviour of such kinds of suspensions have been published on YouTube. Several explanations, such as the formation of hydroclusters [133], the role of granular dilatancy [12], and the order-disorder transition [15] have been proposed over the last two decades. Although these explanations offer a qualitative prediction of continuous shear thickening (CST), none of them reproduces discontinuous shear thickening (DST), i.e. the stress jumps suddenly to a much higher (or infinite) value above a critical shear rate [12]. The cornstarch mentioned above can be regarded as a typical example of DST.

Here we discuss a promising model, proposed by [86] and Wyart and Cates [135], that establishes a deep connection between the rheology of dense suspensions and granular matter and reveals the crucial role of frictional contacts between solid particles. The proposed scenario is the following. At low shear rate, the formation of frictional contacts between particles is inhibited by a short-range repulsive interaction. These repulsive interactions may originate from electrostatics, polymer coatings, or other physics [97]. Therefore, the rheology corresponds to that of a suspension of frictionless particles, indicated by the blue curve in Figure 2.6 B. The viscosity value now can be calculated from Equation 2.28 with $\phi_c = \phi_{RCP} \approx 0.64$. When the shear rate increases, the

particle pressure increases and becomes strong enough to overcome the repulsive force and contribute to the formation of frictional contacts between particles. The rheology switches to that of frictional suspensions, indicated by the red curve in Figure 2.6 B, and the viscosity diverges at a lower critical volume fraction $\phi_c^{\mu_p \neq 0}$. At high volume fraction ($\phi_c^{\mu_p \neq 0} < \phi < \phi_c^{\mu_p = 0}$), the suspension flows like a liquid at low shear rate but suddenly jams when the frictional contacts are triggered at high shear rate since ϕ is larger than the maximum volume fraction for frictional suspensions. This is so-called discontinuous shear thickening (DST).

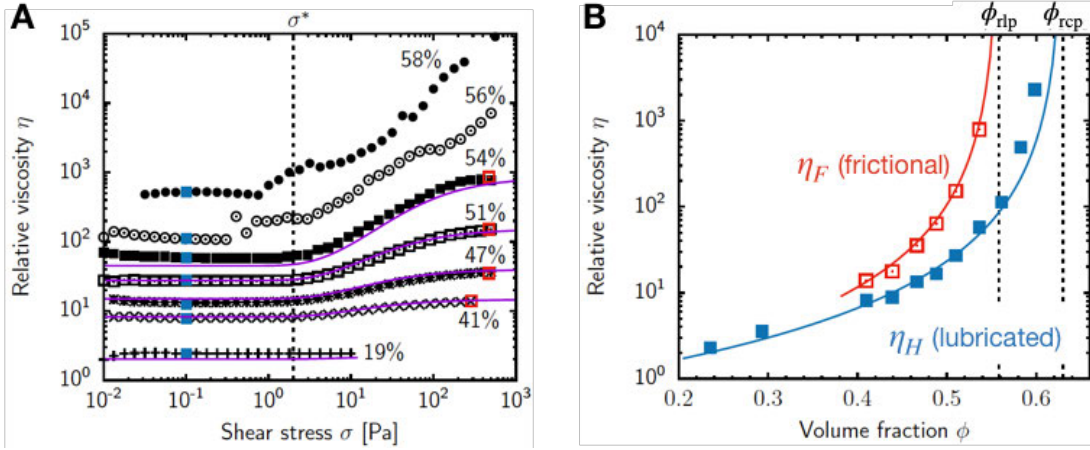


Figure 2.6 (A) Relative viscosity vs shear stress ($\eta_r - \sigma$) for PMMA spheres with average $d = 3.77 \mu\text{m}$. The dashed line indicates the value of onset stress σ_* , and the solid purple line is fitted by the Wyart-Cates theory. (B). Two viscosity branches vary as functions of volume fraction ($\eta_r - \phi$). Corresponding jamming volume fractions, ϕ_{rlp} for frictional particles and ϕ_{rcp} for frictionless particles are indicated by dashed lines. Viscosity values ($\eta_{\text{lubricated}}$) for the lubricated branch are taken from the left lower plateaus of A, indicated by solid blue square in both A and B. Viscosity values ($\eta_{\text{frictional}}$) for the frictional branch are taken from the right higher plateaus of A, indicated by red hollow square in both A and B. Figures are taken and taken from Guy et al. [39].

Based on the stress-controlled transition from frictionless to frictional contacts that give rise to shear thickening, Wyart and Cates [135] proposed an analytical model by making critical volume fraction ϕ_J stress-dependent, i.e. $\phi_J = \phi_J(\sigma)$.

In the Wyart-Cates(WC) model, particle-particle contacts are either frictionless or named as lubricated, which means the real contacts is not formed, with $\mu_p = 0$, or frictional, with $\mu_p > 0$. The fraction of frictional contacts in total contacts, $f(\sigma)$, is controlled by σ . The jamming volume fraction ϕ_J is assumed to be a

linear function of f :

$$\phi_J(f) = f \cdot \phi_{RLP} + (1 - f) \cdot \phi_{RCP} \quad (2.29)$$

According to the equation above, ϕ_J changes linearly from a random loose packing, ϕ_{RLP} , at $f = 1$ to a random close packing, ϕ_{RCP} , at $f = 0$. And the viscosity value of suspension with a given σ , which determines f , can be described by adapting Equation 2.28:

$$\eta(\sigma, \phi) = A \left(1 - \frac{\phi}{\phi_J(\sigma)} \right)^{-2} \quad (2.30)$$

For describing the relationship between f and σ , Guy et al. [39] proposed a ϕ -independent sigmoidal form:

$$f(\sigma) = e^{-(\sigma^*/\sigma)^\beta} \quad (2.31)$$

where σ^* is the onset stress at which $\eta(\sigma)$ visibly starts to increase, indicated by the dashed vertical line in Figure 2.6 A and $\beta = 0.85$ in experiments by Guy et al. [39]. In the discrete element simulations (DEM), Mari et al. [86] proposed a critical load model (CLM) to capture the transition of friction coefficient μ_p of particle contacts from 0 to > 0 when the normal contact force between particles exceeds a threshold value, F^* and successfully reproduced the shear thickening phenomenology. The flow curve of shear thickening is successfully fitted by combining Equation (2.31)(2.29) and (2.30) with $\beta = 1.1$, and $\sigma^* \approx F^* / [6\pi (d_p/2)^2]$. The WC model is widely accepted and supported by different numerical and experimental research [111][20].

2.2.4 Shear-induced migration

Suspensions discussed above are viewed as an effective fluid since the solid particles and the fluid are assumed to move with identical average velocity under simple shear, in which the strain rate field is simple and homogenous. However, the relative motion between the fluid and the particles are inevitable and in many flow configurations [37]. Here we briefly discuss about the shear-induced migration (SIM).

Shear-induced migration is an intriguing phenomenon for suspensions, originally observed in pipe flows by Karnis et al. [57] and in channel flows by Koh et al. [61].

It is the process that particles in suspensions migrate irreversibly from the high-shear-rate region to the low-shear-rate region. For the pressure driven Poiseuille flow, the particles are seen to migrate from the area close to the boundary towards the centreline, where the shear rate is close to 0. For explaining and predicting the shear-induced migration, two types of models have been proposed. A diffusive model proposed by Phillips et al. [106] describes the migration flux by the gradient of the particle concentration and shear rate. This diffusion model successfully predicts the migration in Couette and Poiseuille flows, but fails to predict the absence of migration in curvilinear torsional flows Morris and Boulay [92]. Another phenomenological model called suspension balance model⁶ [100][101][92] relates the migration flux to the divergence of the normal stress of the solid phase. The suspension balance model achieves great success in capturing the shear-induced migration and widely implemented into Eulerian-Eulerian method [78] for simulating industrial processes such as particle separation [114], hydraulic fracture [26] and injection modeling [35].

In this section, we mainly discuss the shear-thickening behaviour, a typical phenomenon influenced by the contact interactions between particles, and shear-induced migration of suspensions, a typical phenomenon influenced by the relative motion between the fluid and solid particles. More complex interactions between particles and geometries will definitely contribute to more interesting and unpredictable issues in the rheology of dense suspensions. A more comprehensive and detailed introduction and review of suspension rheology can be found in Guazzelli and Pouliquen [37]. In this work, we use the discrete element method, which captures the interaction and motion of solid particles, and a coupled lattice Boltzmann method, which captures the fluid field and solid-fluid interactions, to simulate the shear-thickening behaviour and shear-induced migration in the channel flow. An introduction about the discrete element method and the lattice Boltzmann method is presented in the next section.

⁶Details about suspension balance model will be introduced in Chapter 5.

Chapter 3

Numerical methods

This thesis presents a study in which we used a Lattice-Boltzmann coupled discrete element method (DEM) to simulate a suspension system with high solid volume fraction under low Reynolds number conditions. DEM is a versatile and flexible tool for simulating particle systems, capable of capturing a wide range of particle-particle interactions, such as contact forces, collision, and friction. Additionally, it can simulate particles with different shapes, sizes, and surface properties, making it useful for simulating complex particle-fluid interactions.

LBM is a mesoscopic fluid simulation technique that solves the discrete Boltzmann equation at the mesoscale level. This approach is computationally more efficient than solving the Navier-Stokes equations directly in CFD because LBM models the fluid flow in a discrete lattice, which reduces the number of degrees of freedom and computational overhead. In LB-DEM coupling, the fluid and solid phases are separated by a simple bounce-back rule at the lattice nodes, which is much easier to implement and less computationally expensive than the finite-element or finite-volume methods used in CFD-DEM coupling.

In this chapter, we provide a brief introduction to DEM and LBM, as well as the coupling between these two methods. We also present a modification of lubrication forces to account for cases where gap distances between particles are smaller than the resolution of LBM to improve the accuracy of the simulation results for dense suspension systems.

3.1 Discrete Element Method

3.1.1 Basic theory

The discrete element method (DEM), related to molecular dynamics, is a widely used particle-based simulation method in engineering processes. As introduced by Cundall and Strack [21], the translational and rotational motions of particles in the simulation system are determined by solving Newton's second law, considering various kinds of force acting on particles. Thereby, the translational motion is:

$$m_i \frac{d\mathbf{x}_i}{dt} = \mathbf{F}_i^C + \mathbf{F}_i^H + \mathbf{F}_i^* \quad (3.1)$$

and the angular motion:

$$J_i \frac{d\boldsymbol{\omega}_i}{dt} = \mathbf{T}_i^C + \mathbf{T}_i^H + \mathbf{T}_i^* \quad (3.2)$$

where m_i , $\mathbf{x}_i$, J_i and $\boldsymbol{\omega}_i$ are, respectively, the mass, position, moment of inertia and angular velocity of an individual particle i . $\mathbf{F}$ and $\mathbf{T}$ denote the force and the torque acting on each particle, including a mechanical contact ($\mathbf{F}^C$ and $\mathbf{T}^C$) when particles overlap (section 3.1.2), a hydrodynamic interaction ($\mathbf{F}^H$ and $\mathbf{T}^H$) (section 3.1.3), which contains a Stokes drag between particle and fluid and a lubrication interaction ($\mathbf{F}^L$ and $\mathbf{T}^L$) when particles are close to each other resulting in a mutual influence through the surrounding fluid, and other kinds of interaction ($\mathbf{F}^*$ and $\mathbf{T}^*$), e.g. electrostatic interaction, Brownian motion and van der Waals.

3.1.2 Particle contact

The contact between overlapped granular particles can be modelled by a spring-dashpot model [83][45], as shown in Figure 3.1, which contains elastic and damping components:

$$\mathbf{F}^C = \mathbf{F}_e^C + \mathbf{F}_{damping}^C \quad (3.3)$$

For the Hooke model, a linear spring-dashpot model we use in our simulations, the elastic component of the normal force acting on particle i due to the overlap

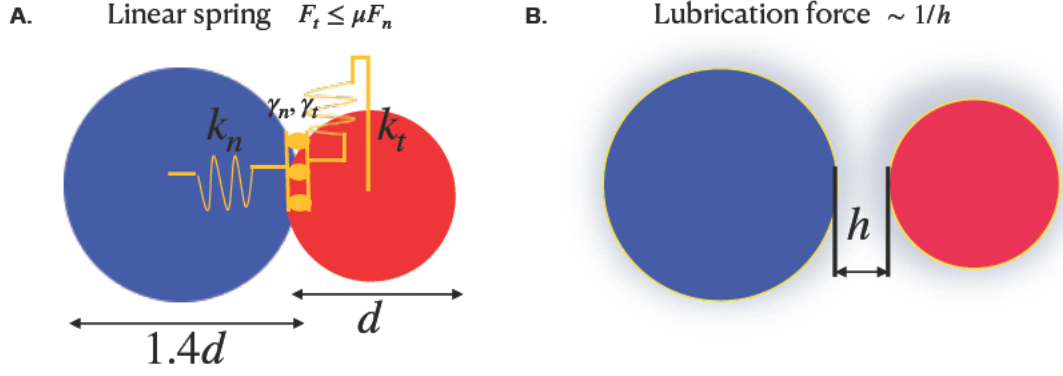


Figure 3.1 Sketches of (A). spring-dashpot model of particle contact (B).lubrication between particles.

δ_{ij} with particle j is given by:

$$\mathbf{F}_{n,e}^C = k_n \delta_{ij} \mathbf{n} \quad (3.4)$$

Here k_n is spring stiffness and $\delta_{ij} = R_i + R_j - \|\mathbf{r}_{ij}\|$ is the particle overlap, R_i, R_j are the radii of particle i and j , $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$ is the vector between two particle centers, and $\mathbf{n} = \frac{\mathbf{r}_{ij}}{\|\mathbf{r}_{ij}\|}$ denotes the direction vector. The direction of the normal force is shown in Figure3.2(A).

The damping component of the normal force is:

$$\mathbf{F}_{n,damp}^C = -\gamma_n \mathbf{u}_{n,rel} \quad (3.5)$$

Here γ_n is the damping coefficient and $\mathbf{u}_{n,rel} = \mathbf{u}_{rel} \cdot \mathbf{n}$ is the normal component of relative velocity between two particles, where $\mathbf{u}_{rel} = \mathbf{u}_i - \mathbf{u}_j$.

Similarly, the tangential component of the particle contact also contains elastic and damping parts, reading:

$$\mathbf{F}_t^C = k_t \delta_t \mathbf{t} + \gamma_t \mathbf{u}_{rel,t} \quad (3.6)$$

where k_t , $\mathbf{t}$, γ_t and $\mathbf{u}_{rel,t}$ are, respectively, spring stiffness, tangential direction vector, as shown in Figure 3.2(A) with opposite direction with relative motion, damping coefficient and relative velocity in the tangential direction, whereas δ_t is a history-dependent tangential displacement, which is accumulated during the

entire duration of the contact:

$$\delta_t = \int_{t_0}^t \mathbf{v}_{t,rel}(\tau) d\tau \quad (3.7)$$

Where $\mathbf{v}_{t,rel}$ is the tangential component of the relative velocity between particles in the contact. δ_t is initialized to 0 and updated following [119]. In our simulations of dense suspension system, the damping coefficients γ_n and γ_t are set to be 0 due to the already existing dissipation provided by lubrication interaction between particles. The tangential spring stiffness k_t is chosen to be $k_t = 2/7k_n$, which ensures similar oscillations of springs in normal and tangential directions, according to the analysis of the oscillation periods conducted by Schäfer et al. [116]. Moreover, the typical response time of Hooke model, a linear spring-dashpot model, which describes particle contacts as damped harmonic oscillators, can be computed analytically[83] by:

$$t_c = \frac{\pi}{\omega} \quad (3.8)$$

where $\omega = \sqrt{(k_{n,t}/m_{ij}) - \eta_{n,t}^2}$ is the eigenfrequency of the contact, the rescaled damping coefficient $\eta_{n,t} = \gamma_{n,t}/(2m_{ij})$ ¹, and the reduced mass $m_{ij} = m_i m_j / (m_i + m_j)$. The integration timestep Δt_{DEM} in DEM should be much smaller than t_c , i.e. $\Delta t_{DEM} \ll t_c$ to make sure particle motions described by Equation 3.1 and Equation 3.2 are stable. Besides, the inertial relaxation time and viscous relaxation time play an important role in DEM simulations of suspensions, as highlighted in Section 2.2.1. In the context of Stokes flow (i.e., low shear rate $\dot{\gamma}$ and low Reynolds number) and stiff particles (i.e., large particle stiffness k_n), both the inertial relaxation time and viscous relaxation time are orders of magnitude larger than t_c .

Additionally, friction also plays an important role in the simulation of granular particles. Therefore, the maximum friction force in the tangential direction $\mathbf{F}_t^C$ should satisfy the Coulomb friction criterion:

$$|\mathbf{F}_t^C| \leq \mu_p |\mathbf{F}_n^C| \quad (3.9)$$

where μ_p is the friction coefficient between particles in contact. According to the limitation of friction force, the tangential force should be $\mathbf{F}_t^C = \min(k_t \delta_t, \mu |\mathbf{F}_n^C|) \mathbf{t}$, where the damping component is neglected since γ_t is set to be 0 in our simulation as mentioned before. Friction described here specifically refers to sliding friction,

¹Here the subscripts n, t denote the components in normal and tangential directions, respectively.

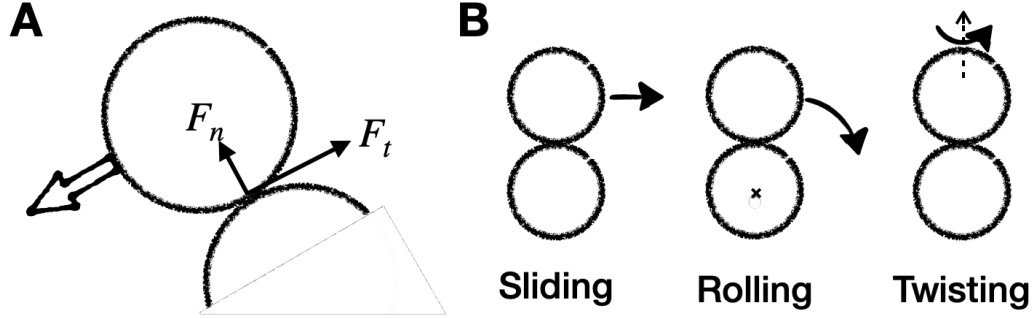


Figure 3.2 Sketches of (A) contact force of normal and tangential directions in DEM simulations (B) different types of constraints for particles in contact

as it only provides resistance in the tangential motion of particles.

Besides the aforementioned contact models, many other models are also proposed to include different properties of granular particles, such as the adhesive model proposed by Luding [83] for describing a plastic(hysteretic) effect when particles get into contact and the bond model proposed by Brown et al. [13] for describing deformable structures. Meanwhile, similar to the aforementioned sliding friction, the rolling friction, which resists the pure rolling motion of particles and twisting friction, which resists the rotation of two contacting particles about the normal direction $\mathbf{n}$, as shown in Figure 3.2(B), are also taken into consideration in many pieces of research[121][110][40]. A detailed discussion is not carried out here, and we only consider spherical particles modelled by a linear spring model with sliding friction in our simulations so far.

More detailed information about the granular contact model can be found in the granular section of LAMMPS documentation.

3.1.3 Hydrodynamic interactions

The motion of particles immersed in a fluid will be influenced by hydrodynamic interactions, which contain two parts: resisting force from the relative motion between a single particle and fluid, i.e. Stokes drag as shown in Figure 3.3(A), and lubrication force, provided by the interstitial fluid, resulting from the relative motion of a pair of, or more, particles[36].

Stokes drag

Particles immersed in a viscous background fluid will feel resistance forces, also called drag forces in fluid dynamics. For low Reynolds number, where Stokes' law holds, the drag force acting on a small spherical particle moving through a viscous laminar flow can be derived as:

$$\mathbf{F}_{\text{Stokes}} = 6\pi\eta_f r_p (\mathbf{u}_f^\infty(\mathbf{x}_p) - \mathbf{u}_p) \quad (3.10)$$

$$\mathbf{T}_{\text{Stokes}} = 8\pi\eta_f r_p (\boldsymbol{\omega}_f^\infty(\mathbf{x}_p) - \boldsymbol{\omega}_p) \quad (3.11)$$

Here η_f and r_p are the fluid dynamic viscosity and particle radius, respectively. The fluid rotation is $\boldsymbol{\omega}^\infty(\mathbf{x}_p) = \frac{1}{2}(\nabla \times \mathbf{u}_f^\infty(\mathbf{x}_p))$. Here we use the notation $\mathbf{u}_f^\infty(\mathbf{x})$ to indicate the velocity field without any disturbance due to the particles, so do other quantities, such as the rotation $\boldsymbol{\omega}^\infty$ and strain tensor $\mathbf{E}^\infty$. Specifically, for an imposed simple shear flow with a shear rate $\dot{\gamma}$, as shown in Figure 3.3(A), a linear fluid velocity profile can be assumed, i.e. $E_{xy}^\infty = E_{yx}^\infty = \dot{\gamma}/2$ and $\Omega_z^\infty = \dot{\gamma}/2$.

The presence of other particles in a fluid suspension can impact the drag force acting on a single sphere, resulting in a reduction in the effective viscosity of the fluid. A common approach to account for this effect is by introducing a hindrance function, which is described in detail in Section 6.1.1. However, our DEM approaches have already incorporated pairwise lubrication interactions and contacts between particles, which implicitly account for the influence of other particles on the particle motion. As such, we calculate the drag forces acting on individual particles using the conventional Stokes drag law for a single sphere, rather than a modified drag force based on a hindrance function.

Lubrication

For dense suspensions where the surface separation between particles is sufficiently small, compared to particle size, the lubrication effects between particles become dominant as a result of large gap pressure [36]. Instead of considering the many-body nature of the full, long-range hydrodynamic interactions, lubrication effects are introduced as a pair-wise short-range interaction with a threshold, which is the ratio of gap distance and particle size ($h_{\text{threshold}}/r_p$) and denoted as

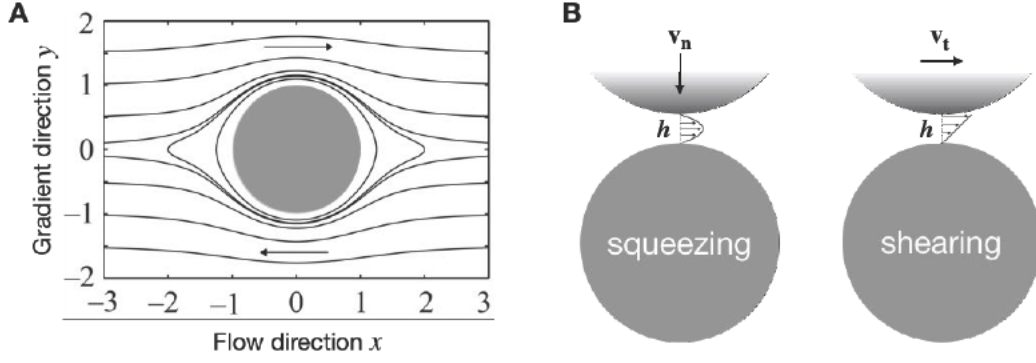


Figure 3.3 A. Schematic 2D profile of streamline around a sphere under simple shear flow. B. Squeezing and shearing lubrication hydrodynamics. Both adapted from Guazzelli and Morris [36].

$\delta_{o,c}^2$, of gap distance between particles in pair. As shown in Figure 3.3(B), for two spheres in a relative translation with velocity $\mathbf{v}_n$ along their line of centres, the normal (squeeze) lubrication force acting on the spheres is:

$$\mathbf{F}_{sq} \sim -\eta_f r_p^2 \mathbf{v}_n h^{-1} \quad (3.12)$$

where h is the gap distance and $h \ll r_p$. $\mathbf{F}_{sq}$ diverges as $1/h$. For the relative velocity $\mathbf{v}_t$ perpendicular to the normal direction, the tangential (shear) lubrication force is:

$$\mathbf{F}_{sh} \sim -\eta_f r_p^2 \mathbf{v}_t \ln h \quad (3.13)$$

which diverges much more weakly than the squeeze force.

More detailed lubrication interaction between two particles can be expressed in a grand-resistance matrix (GRM) [52][58] notation as:

$$\begin{pmatrix} \mathbf{F}_1 \\ \mathbf{F}_2 \\ \mathbf{T}_1 \\ \mathbf{T}_2 \\ \mathbf{S}_1 \\ \mathbf{S}_2 \end{pmatrix} = \eta_f \begin{pmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} & \tilde{\mathbf{B}}_{11} & \tilde{\mathbf{B}}_{12} & \tilde{\mathbf{G}}_{11} & \tilde{\mathbf{G}}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} & \tilde{\mathbf{B}}_{21} & \tilde{\mathbf{B}}_{22} & \tilde{\mathbf{G}}_{21} & \tilde{\mathbf{G}}_{22} \\ \mathbf{B}_{11} & \mathbf{B}_{12} & \mathbf{C}_{11} & \mathbf{C}_{12} & \tilde{\mathbf{H}}_{11} & \tilde{\mathbf{H}}_{12} \\ \mathbf{B}_{21} & \mathbf{B}_{22} & \mathbf{C}_{21} & \mathbf{C}_{22} & \tilde{\mathbf{H}}_{11} & \tilde{\mathbf{H}}_{12} \\ \mathbf{G}_{11} & \mathbf{G}_{12} & \mathbf{H}_{11} & \mathbf{H}_{12} & \mathbf{M}_{11} & \mathbf{M}_{12} \\ \mathbf{G}_{21} & \mathbf{G}_{22} & \mathbf{H}_{21} & \mathbf{H}_{22} & \mathbf{M}_{21} & \mathbf{M}_{22} \end{pmatrix} \cdot \begin{pmatrix} \mathbf{v}^\infty(\mathbf{x}_1) - \mathbf{u}_{p,1} \\ \mathbf{v}^\infty(\mathbf{x}_2) - \mathbf{u}_{p,2} \\ \boldsymbol{\omega}^\infty - \boldsymbol{\omega}_{p,1} \\ \boldsymbol{\omega}^\infty - \boldsymbol{\omega}_{p,2} \\ \mathbf{E}^\infty \\ \mathbf{E}^\infty \end{pmatrix} \quad (3.14)$$

The tensor elements in the resistance matrix determine the force on one particle in dependence on itself and the other particle. The details of the GRM evaluation

²Here o, c is the abbreviation of outer cutoff

and the final expressions for force and torque, which were implemented into LIGGGHTS, an open source DEM project [60], by my colleague Tim Najuch. The simplifications were derived by my colleague Rangarajan Radhakrishnan [108] and implemented into LIGGGHTS and LAMMPS, an open source DEM project [128]. The simplified expressions read as:

$$\mathbf{F} = \eta_f \left[X_A^{11} \mathbf{u}_{p,rel,n} + Y_A^{11} (\mathbf{u}_{p,rel,t} - (r_{p,1} + r_{p,2}) (\boldsymbol{\omega}_s \times \mathbf{e})) + \frac{1 - \beta(1 + 4\beta)}{4 + \beta} Y_B^{11} (\boldsymbol{\omega}_d \times \mathbf{e}) \right] \quad (3.15)$$

$$\mathbf{T} = \eta_f \left[Y_B^{11} (\mathbf{u}_{p,rel} \times \mathbf{e}) + (r_{p,1} + r_{p,2}) (\boldsymbol{\omega}_s - (\boldsymbol{\omega}_s \cdot \mathbf{e}) \mathbf{e}) + Y_C^{12} \left(1 - \frac{4}{\beta} \right) (\boldsymbol{\omega}_d - (\boldsymbol{\omega}_d \cdot \mathbf{e}) \mathbf{e}) \right] \quad (3.16)$$

where $\boldsymbol{\omega}_s = (\boldsymbol{\omega}_{p,1} + \boldsymbol{\omega}_{p,2})/2$, $\boldsymbol{\omega}_d = (\boldsymbol{\omega}_{p,1} - \boldsymbol{\omega}_{p,2})/2$, and $\mathbf{u}_{p,rel,n}$ and $\mathbf{u}_{p,rel,t}$ are the normal and tangential components of the relative velocity $\mathbf{u}_{p,rel} = \mathbf{u}_{p,2} - \mathbf{u}_{p,1}$ between particles 1 and 2. β is the size ratio between particles 1 and 2. In the simplified expression of the force, the three terms represent lubrication forces caused by normal squeeze, tangential shear and relative rotation. For the expression of the torque, the two terms are caused by tangential shear and relative rotation, respectively. The resistance functions X_A^{11} , Y_A^{11} , Y_B^{11} , and Y_C^{12} are taken to the order of $\log(\xi^{-1})$ with $\xi = \frac{h}{r_p}$ from Kim and Karrila [58].

As previously discussed, the lubrication forces between particles result in a divergence as the gap distance between particle surfaces approaches zero. However, in reality, particle surfaces are not perfectly smooth, and contact between particles may occur due to the influence of surrounding particles and the Stokes flow. To account for this phenomenon, we introduce an inner cutoff distance into the lubrication models. This cutoff accounts for the effects of surface roughness and the breakdown of the lubrication force as the gap distance approaches the typical scaling of surface roughness. By introducing this inner cutoff, we can accurately describe particles overcoming the lubrication film and coming into the mechanical contact.

In our DEM simulations, we choose $\delta_{c,o} = 0.1$ and $\delta_{c,i} = 0.001$, i.e. lubrication forces are 0 when gap distances between particles are larger than $0.1d_p$, and stay constant when gap distances are smaller than $0.001d_p$.

As discussed above, the hydrodynamic force acting on particles in DEM

simulations contains a contribution from the Stokes drag and a contribution from the pair-wise short-range lubrication force. However, the fluid flow is also disturbed by the particle motion, which makes the expression of Stokes drag, as shown in Equation(3.10), unreliable, such as the shear migration in pressure-driven flow. Therefore, a resolved fluid field around the particles is required, and a lattice Boltzmann method (LBM) is introduced for coupling with DEM [2].

3.2 Lattice-Boltzmann Method

The lattice Boltzmann method (LBM) originated from the lattice gas automata (LGA) method³, is a class of computational fluid dynamics (CFD) methods for complex fluid simulations. Instead of solving macroscopic continuum equations (Navier-Stokes equations) directly, the lattice Boltzmann method simulates macroscopic dynamics of a fluid by constructing a simplified fictitious molecular dynamics model, which provides many advantages, including clear physical pictures, easy implemented boundary conditions and straightforward parallel algorithms[17]. With the rapid development in the last three decades, LBM has been proven to be an efficient and convenient alternative to traditional CFD methods for a large variety of industrial and physical problems[112][63][74] like porous media flows[17], particle-fluid suspensions[66] and flows of polymer solvent systems[1].

3.2.1 Boltzmann equation

In 1872, Ludwig Boltzmann proposed the Boltzmann equation, or Boltzmann transport equation, to describe the statistical behavior of a thermodynamic system out of equilibrium. The Boltzmann equation reads:

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial f}{\partial \mathbf{x}} + \frac{\mathbf{F}}{m} \cdot \frac{\partial f}{\partial \boldsymbol{\xi}} = \left(\frac{\partial f}{\partial t}\right)_{coll} \quad (3.17)$$

In the equation, $\mathbf{x}$, $\boldsymbol{\xi}$ and m are, respectively, the position, velocity and mass of liquid molecules. $\mathbf{F}$ is the force field acting on the particles. And f , related to $(\mathbf{x}, \boldsymbol{\xi}, t)$, is the probability density function that provides information about

³LBM was originally introduced by McNamara and Zanetti [87] from LGA. Here we would not talk about LGA in detail, and related information can be easily found in Chen and Doolen [17], Krüger et al. [63] and many other pieces of literature

molecules which all have velocity $\boldsymbol{\xi}$ and position $\boldsymbol{x}$ within a differential volume element $d\boldsymbol{x}d\boldsymbol{\xi}$ of a phase space $(\boldsymbol{x}, \boldsymbol{\xi})^4$ at specific time t . Thus the number of molecules within such a volume element is:

$$dN = f(\boldsymbol{x}, \boldsymbol{\xi}, t)d\boldsymbol{x}d\boldsymbol{\xi} \quad (3.18)$$

By integrating over the whole phase space, the number of molecules can be calculated by:

$$N = \int_{\boldsymbol{\xi}} \int_{\boldsymbol{x}} f(\boldsymbol{x}, \boldsymbol{\xi}, t)d\boldsymbol{x}d\boldsymbol{\xi} \quad (3.19)$$

We can also get the macroscopic density and momentum in a similar way:

$$\rho(\boldsymbol{x}, t) = \int f(\boldsymbol{x}, \boldsymbol{\xi}, t)d^3\boldsymbol{\xi} \quad (3.20)$$

$$\rho(\boldsymbol{x}, t)\boldsymbol{u}(\boldsymbol{x}, t) = \int f(\boldsymbol{x}, \boldsymbol{\xi}, t)\boldsymbol{\xi}d^3\boldsymbol{\xi} \quad (3.21)$$

The left-hand side of the Boltzmann equation Equation(3.17) is related to the evolution of the particle itself, whereas the right-hand side describes the effect of collisions between particles. The approach to modeling the collision term suggested by Boltzmann (1872) is based on the assumption that the collisions are solely between two elastic particles that are uncorrelated prior to the collision, which is known as the "molecular chaos assumption". The derivation of the collision term can be found in Boltzmann [8] and Lieberman and Lichtenberg [79] and the integral can be written as [79]:

$$\left(\frac{\partial f}{\partial t}\right)_{\text{coll}} = \int d^3v_2 \int_0^{2\pi} d\phi_1 \int_0^\pi (f'_1 f'_2 - f_1 f_2) |\boldsymbol{v}_1 - \boldsymbol{v}_2| I \sin \theta_1 d\theta_1 \quad (3.22)$$

where the relative velocity between two particles is $|\boldsymbol{v}_1 - \boldsymbol{v}_2|$ and f_1, f_2 and f'_1, f'_2 are the distribution functions of two particles getting into collision before and after the collision. The integration is performed over all velocities $\boldsymbol{v}_2$, as well as over ϕ_1 and θ_1 , which are azimuthal and polar angles characterizing $\boldsymbol{v}_1 - \boldsymbol{v}_2$, respectively. The collision integral I represents the probability per unit time per unit volume that particles with velocities $\boldsymbol{v}_1$ and $\boldsymbol{v}_2$ in a given direction will collide, and it depends on the interaction forces between the particles. The factor $|\boldsymbol{v}_1 - \boldsymbol{v}_2|$ represents the relative speed of the two particles before the collision. The factor $\sin \theta_1$ represents the solid angle element at which the two particles

⁴The phase space has 6 dimensions $(x, y, z, \xi_x, \xi_y, \xi_z)$ in 3D space and 4 dimensions (x, y, ξ_x, ξ_y) in 2D plane

approach each other, and the integration over θ_1 and ϕ_1 corresponds to averaging over all possible relative orientations of the two particles.

Due to the complexity of the collision term, lots of attempts have been made to simplify the collision term. The most well-known model, named as Bhatnagar-Gross-Krook (BGK) model, was proposed by Bhatnagar et al. [6]:

$$\left(\frac{\partial f}{\partial t}\right)_{coll} = \frac{f^{eq} - f}{\tau(v)} \quad (3.23)$$

The right-hand side of the equation describes that the distribution function f is relaxed towards the local equilibrium distribution function f^{eq} under the effect of a molecular collision over a collision relaxation time τ , which is related to the fluid viscosity. The equilibrium function f^{eq} follows the Maxwell-Boltzmann distribution for identical classical particles:

$$f^{eq}(\mathbf{x}, \boldsymbol{\xi}, t, \mathbf{u}) = \rho \left(\frac{1}{2\pi RT} \right)^{d/2} e^{-(\boldsymbol{\xi} - \mathbf{u})^2 / (2RT)} \quad (3.24)$$

where ρ , $\mathbf{u}$ are the macroscopic fluid density and velocity, respectively. d is the number of spatial dimensions. R and T are the gas constant and the temperature, respectively.

3.2.2 Discretised Boltzmann equation

The Boltzmann equation (Equation(3.17)), introduced in the previous section, is difficult to solve analytically as it spans over seven dimensions ($x, y, z, \xi_x, \xi_y, \xi_z$ and t) for 3D space, whereas we can solve the Boltzmann equation numerically and therefore a discretisation for velocity space, physical space and time is required. Here we just briefly talk about the procedure of discretisation, and the detailed elucidation can be found in Succi [125] and Krüger et al. [63].

Nondimensionalization Nondimensionalization is the first step in Lattice Boltzmann method(LBM) and can be accomplished by introducing following scales[71][2]: characteristic length scale L_s , characteristic velocity U_s and reference density ρ_s . Hence, some nondimensional quantities can be obtained through basic

dimensional analysis:

$$\begin{array}{ll}
\text{Time} & \hat{t} = \frac{tU_s}{L_s} \\
\text{Length} & \hat{\mathbf{r}} = \frac{\mathbf{r}}{L_s} \\
\text{Density} & \hat{\rho} = \frac{\rho}{\rho_s} \\
\text{Macroscopic velocity} & \hat{\mathbf{u}} = \frac{\mathbf{u}}{U_s} \\
\text{Reynolds number} & \text{Re} = \frac{U_s L_s}{\nu}
\end{array} \tag{3.25}$$

Discretisation in space and time

The discretisations of the Boltzmann equation in space and time are quite straightforward by applying common numerical techniques, where Δx is the basic unit for lattice spacing and Δt is the basic unit of the time step, which represent a spatial resolution and a time resolution, respectively. The lattice spacing Δx and time step Δt here can serve as the characteristic scales for LBM, as we discussed above.

Discretisation in velocity space

Given the exponential form of the equilibrium distribution function f^{eq} , as shown in Equation(3.24), Hermite polynomials are employed for the expansion and discretisation of f^{eq} because of the similar exponential form of weighting function, $\omega(x) = \frac{1}{(2\pi)^{d/2}} e^{-x^2/2}$, of Hermite polynomials. Now the equilibrium distribution function, Equation(3.24), can be expanded as⁵:

$$f^{eq}(\rho, \mathbf{u}, \theta, \boldsymbol{\xi}) = \omega(\boldsymbol{\xi}) \sum_{n=0}^{\infty} \frac{1}{n!} \mathbf{a}^{(n),eq}(\rho, \mathbf{u}, \theta) \cdot \mathbf{H}^{(n)}(\boldsymbol{\xi}) \tag{3.26}$$

and

$$\mathbf{a}^{(n),eq}(\rho, \mathbf{u}, \theta) = \int f^{eq}(\rho, \mathbf{u}, \theta, \boldsymbol{\xi}) \mathbf{H}^{(n)}(\boldsymbol{\xi}) d^d \boldsymbol{\xi} = \frac{\rho}{\theta^{d/2}} \int \omega\left(\frac{\boldsymbol{\xi} - \mathbf{u}}{\sqrt{\theta}}\right) \mathbf{H}^{(n)}(\boldsymbol{\xi}) d^d \boldsymbol{\xi} \tag{3.27}$$

⁵detailed derivation can be found in Chapter3 of Krüger et al. [63]

where $\mathbf{H}^{(n)}$ is nth Hermite polynomial (see in Appendix A) and $\theta = RT$. And we can get the following:

$$\begin{aligned} a^{(0),eq} &= \rho \\ a_{\alpha}^{(1),eq} &= \rho u_{\alpha} \\ a_{\alpha\beta}^{(2),eq} &= \rho (u_{\alpha} u_{\beta} + (\theta - 1) \delta_{\alpha\beta}) \\ a_{\alpha\beta\gamma}^{(3),eq} &= \rho [u_{\alpha} u_{\beta} u_{\gamma} + (\theta - 1) (\delta_{\alpha\beta} u_{\gamma} + \delta_{\beta\gamma} u_{\alpha} + \delta_{\gamma\alpha} u_{\beta})] \end{aligned} \quad (3.28)$$

We can find that the first three terms of the Hermite series expansion correspond to density, momentum and energy, which means these three terms are sufficient to capture the macroscopic physics. Now f^{eq} can be approximated up to the second order ($N = 2$):

$$\begin{aligned} f^{eq}(\rho, \mathbf{u}, \theta, \boldsymbol{\xi}) &\approx \omega(\xi) \rho [1 + \xi_{\alpha} u_{\alpha} + (u_{\alpha} u_{\beta} + (\theta - 1) \delta_{\alpha\beta}) (\xi_{\alpha} \xi_{\beta} - \delta_{\alpha\beta})] \\ &= \omega(\xi) \rho Q(\mathbf{u}, \theta, \boldsymbol{\xi}) \end{aligned} \quad (3.29)$$

where $Q(\mathbf{u}, \theta, \boldsymbol{\xi})$ is a multi-dimensional polynomial in $\boldsymbol{\xi}$.

According to the *Gauss-Hermite quadrature rule*:

$$\int \omega(x) P^{(N)}(x) d^d x = \sum_{i=1}^n w_i P^{(N)}(\mathbf{x}_i) \quad (3.30)$$

where the certain point $\mathbf{x}_i$ is a root of $H^{(n)}(x_i) = 0$, we can get discretized form of $\mathbf{a}^{(n),eq}$ from Equation(3.27) and Equation(3.29):

$$a^{(n),eq} = \int f^{eq}(\boldsymbol{\xi}) \mathbf{H}^{(n)}(\boldsymbol{\xi}) d^d \xi = \rho \int \omega(\boldsymbol{\xi}) Q(\boldsymbol{\xi}) \mathbf{H}^{(n)}(\boldsymbol{\xi}) d^d \xi = \rho \sum_{i=1}^n w_i Q(\boldsymbol{\xi}_i) \mathbf{H}^{(n)}(\boldsymbol{\xi}_i) \quad (3.31)$$

and we can obtain a finite set of $f_i^{eq} = f^{eq}(\boldsymbol{\xi}_i)$:

$$f_i^{eq} = w_i \rho \left[1 + \xi_{i\alpha} u_{\alpha} + \frac{1}{2} (u_{\alpha} u_{\beta} + (\theta - 1) \delta_{\alpha\beta}) (\xi_{i\alpha} \xi_{i\beta} - \delta_{\alpha\beta}) \right] \quad (3.32)$$

Based on the discussion above, the final form of the discrete equilibrium distribution function reads:

$$f_i^{eq} = w_i \rho \left(1 + \frac{c_{i\alpha} u_{\alpha}}{c_s^2} + \frac{u_{\alpha} u_{\beta} (c_{i\alpha} c_{i\beta} - c_s^2 \delta_{\alpha\beta})}{2c_s^4} \right) \quad (3.33)$$

Here $\mathbf{c}_i = \frac{\boldsymbol{\xi}_i}{\sqrt{3}}$. c_s is the speed of sound. The isothermal assumption implies $\theta = 1$

to remove the temperature from the equilibrium distribution.

The particle distribution function f can be discretised in the same procedure. Now the dimensionless and velocity-discretised Boltzmann equation reads:

$$\frac{\partial f_i}{\partial t} + \mathbf{c}_{i,\alpha} \cdot \frac{\partial f_i}{\partial \mathbf{x}_\alpha} = \Omega(f_i) \quad (3.34)$$

where Ω is the collision term, which corresponds to Equation 3.23 under the BGK approximation.

The macroscopic density and momentum can be calculated from the following:

$$\begin{aligned} \rho &= \sum_i f_i = \sum_i f_i^{\text{eq}} \\ \rho \mathbf{u} &= \sum_i f_i \mathbf{c}_i = \sum_i f_i^{\text{eq}} \mathbf{c}_i \end{aligned} \quad (3.35)$$

Velocity sets

The procedure of discretisation of velocity space by Gauss-Hermite polynomials has been shown in the previous section, and appropriate velocity sets $\mathbf{c}_i$ with corresponding weight sets ω_i are required. The construction of velocity sets has to fulfil the following requirements:

- Conservation of mass, momentum and energy, i.e. based on the Gauss-Hermite quadrature rule described above.
- Rotational isotropy of the lattice.
- All weights ω_i should be non-negative.

Based on the requirements above, Qian et al. [107] proposed the DnQm sets, which means m velocities in n dimensions. The DnQm set has become a widely used discretisation scheme in LBM, including D2Q9 for 2D, D3Q15, D3Q19 and D3Q27 for 3D.

D2Q9 and D3Q27 The velocity sets for D2Q9 and D3Q19 are shown in Figure 3.4 and explicit velocity sets ω_i, c_i for D2Q9 and D3Q19 can be found in Table 3.1 and Table 3.2. D2Q9 is the two-dimensional velocity set, and easier

for us to understand the boundary condition in the later discussion, and D3Q19 is what we use in our simulation. Detailed information about D3Q15 and D3Q27 can be found in Krüger et al. [63].

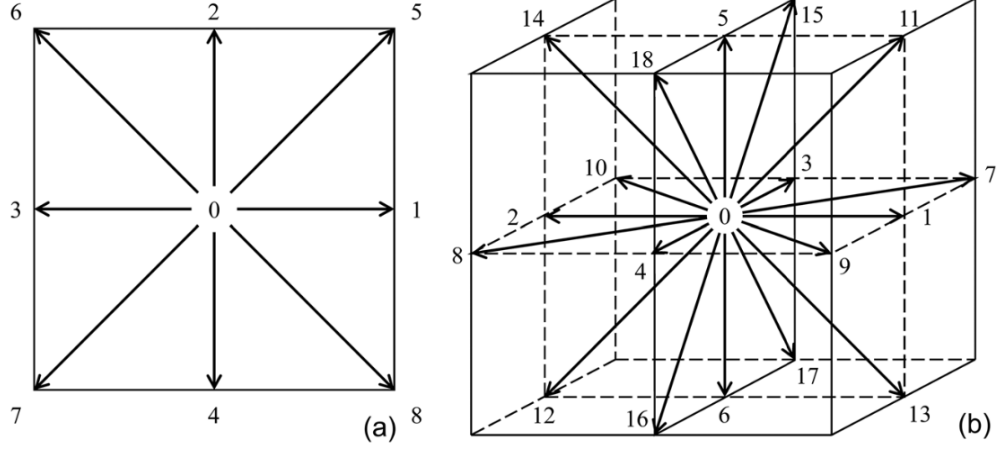


Figure 3.4 (a) 9 velocity vectors in two-dimension plane (b) 19 velocity vectors in three-dimension space(D3Q19). Vector 0 points from centre to centre of the square in 2D and cube in 3D. Figure is taken from Liu and Wu [80]

i	0	1	2	3	4	5	6	7	8
w_i	$\frac{4}{9}$	$\frac{1}{9}$	$\frac{1}{9}$	$\frac{1}{9}$	$\frac{1}{9}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$
c_{ix}	0	+1	0	-1	0	+1	-1	-1	+1
c_{iy}	0	0	+1	0	-1	+1	+1	-1	-1

Table 3.1 The D2Q9 velocity set in explicit form, taken from Krüger et al. [63].

i	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
w_i	$\frac{1}{3}$	$\frac{1}{18}$	$\frac{1}{18}$	$\frac{1}{18}$	$\frac{1}{18}$	$\frac{1}{18}$	$\frac{1}{18}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$
c_{ix}	0	+1	-1	0	0	0	0	+1	-1	+1	-1	0	0	+1	-1	+1	-1	0	0
c_{iy}	0	0	0	+1	-1	0	0	+1	-1	0	0	+1	-1	-1	+1	0	0	+1	-1
c_{iz}	0	0	0	0	0	+1	-1	0	0	+1	-1	+1	-1	0	0	-1	+1	-1	+1

Table 3.2 The D3Q19 velocity set in explicit form, taken from Krüger et al. [63].

Lattice Boltzmann equation

With the discretisation of time, space and velocity space(7 dimensions in total) and the choice of an appropriate velocity set DnQm, we can convert

the continuous Boltzmann equation (Equation(3.17)) to the lattice Boltzmann equation:

$$f_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) = f_i(\mathbf{x}, t) + \Omega_i \Delta t + \mathbf{F}_i \Delta t \quad (3.36)$$

Hence we employ the Bhatnagar-Gross-Krook (BGK) collision operator as mentioned in equation (3.23) for substituting the collision term Ω_i and temporarily ignore the external force term $\mathbf{F}_i$ in equation (3.36), we can get the lattice Boltzmann equation with BGK collision operator, also called the LBGK equation:

$$f_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) = f_i(\mathbf{x}, t) - \frac{\Delta t}{\tau} (f_i(\mathbf{x}, t) - f_i^{\text{eq}}(\mathbf{x}, t)) \quad (3.37)$$

where τ is the dimensionless relaxation parameter and the equilibrium distribution function $f_i^{\text{eq}}(\mathbf{x}, t)$ is:

$$f_i^{\text{eq}}(\mathbf{x}, t) = w_i \rho \left(1 + \frac{\mathbf{u} \cdot \mathbf{c}_i}{c_s^2} + \frac{(\mathbf{u} \cdot \mathbf{c}_i)^2}{2c_s^4} - \frac{\mathbf{u} \cdot \mathbf{u}}{2c_s^2} \right) \quad (3.38)$$

where w_i is the weight specific to the chosen velocity set. ρ and $\mathbf{u}$ are, respectively, the macroscopic fluid density and velocity, determined by:

$$\begin{aligned} \rho &= \sum_i f_i \\ \rho \mathbf{u} &= \sum_i f_i \mathbf{c}_i \end{aligned} \quad (3.39)$$

and $c_s = c/\sqrt{3}$ is the lattice sound speed where $c = \Delta x/\Delta t$ is the lattice speed. The fluid pressure field p is determined by the relationship: $p = c_s^2 \rho$. The fluid kinematic ν is determined by the discretisation and numerical parameters for recovering the Navier-Stokes equation:

$$\nu = \frac{1}{3} \left(\tau - \frac{1}{2} \right) \frac{(\Delta x)^2}{\Delta t} \quad (3.40)$$

Collision and Streaming The LBGK equation (Equation(3.37)) can be decomposed into two distinct parts that are performed in succession:

- collision(or relaxation) part: $f_i^*(\mathbf{x}, t) = f_i(\mathbf{x}, t) - \frac{\Delta t}{\tau} (f_i(\mathbf{x}, t) - f_i^{\text{eq}}(\mathbf{x}, t))$
- streaming(or propagation) part: $f_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) = f_i^*(\mathbf{x}, t)$

So that the lattice Boltzmann equation, equation (3.36) can be understood as

two parts: local collision and non-local propagation from node 0 to neighbouring nodes as shown in Figure 3.4(A).

External force

For the external force term, Guo et al. [38] proposed a modification expression based on the most simple approach, $F_i = \frac{w_i \mathbf{c}_i \mathbf{F}}{c_s^2}$, proposed by He et al. [44], to recover the correct form of the macroscale Navier-Stokes equation with an external force. The modified external force term is:

$$F_i = \left(1 - \frac{1}{2\tau}\right) w_i \left[\frac{\mathbf{c}_i - \mathbf{u}}{c_s^2} + \frac{(\mathbf{c}_i \cdot \mathbf{u})}{c_s^4} \mathbf{c}_i \right] \cdot \mathbf{F} \quad (3.41)$$

and the macroscopic fluid velocity in equation (3.39) has to be modified as:

$$\rho \mathbf{u} = \sum_i f_i \mathbf{c}_i + \frac{\Delta t}{2} \mathbf{F} \quad (3.42)$$

where $\mathbf{F}$ is the macroscale external force. The most straightforward application for such external force in LBM is the simulation of Poiseuille flow driven by a pressure gradient together with a body force, which usually serves as a validation case in many papers [38][80] and becomes a widely used sample case in the tutorials of LBM projects like Palabos[74] and openlb [65].

Collision terms

The BGK model discussed above for simplifying the collision term of the Boltzmann equation is quite straightforward and with great efficiency and simplicity, whereas such single-parameter approximation sacrifices stability and accuracy in some specific conditions, e.g. stability decreases for simulations with large Reynolds number or small viscosity (i.e. $\tau - 1/2$ is close to 0).

To improve the accuracy and stability of LBM simulations, especially for the collision step, multiple relaxation parameters, which can provide more degrees of freedom, rather than one single relaxation parameter, which is related to the viscosity, are introduced to reconstruct collision operators. Here we will briefly discuss the multiple-relaxation-time (MRT) model[70][24] and the two-relaxation-time (TRT) model[34]. There are other methods like the regularised collision operator[72] and entropic collision operators[91], but it is beyond the topic of our

discussion, and we use the common BGK model in our LBDEM simulation.

MRT The basic idea of the MRT model is to relax the macroscale moments instead of the distribution function with individual rates, i.e. individual relaxation parameter ω_i . For this purpose, the particle distribution functions f_i have to be transformed to moment space with a transformation matrix, denoted as $\mathbf{M}$. After performing the collision step in moment space, the moments have to be transformed back to the particle distribution function with $\mathbf{M}^{-1}$.

Based on this idea, we can rewrite the LBGK equation, Equation(3.37) as:

$$\begin{aligned}
\mathbf{f}(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) - \mathbf{f}(\mathbf{x}, t) &= -\omega (\mathbf{f}(\mathbf{x}, t) - \mathbf{f}^{\text{eq}}(\mathbf{x}, t)) \Delta t \\
&= -\mathbf{M}^{-1} \mathbf{M} \omega [\mathbf{f}(\mathbf{x}, t) - \mathbf{f}^{\text{eq}}(\mathbf{x}, t)] \Delta t \\
&= -\mathbf{M}^{-1} \omega [\mathbf{M} \mathbf{f}(\mathbf{x}, t) - \mathbf{M}^{\text{eq}}(\mathbf{x}, t)] \Delta t \quad (3.43) \\
&= -\mathbf{M}^{-1} \omega \mathbf{I} [\mathbf{m}(\mathbf{x}, t) - \mathbf{m}^{\text{eq}}(\mathbf{x}, t)] \Delta t \\
&= -\mathbf{M}^{-1} \mathbf{S} [\mathbf{m}(\mathbf{x}, t) - \mathbf{m}^{\text{eq}}(\mathbf{x}, t)] \Delta t.
\end{aligned}$$

where $\mathbf{I} = \mathbf{M}^{-1} \mathbf{M}$, which ensures that the equivalence relationship holds, and $\mathbf{m}(\mathbf{x}, t) - \mathbf{m}^{\text{eq}}(\mathbf{x}, t)$ describes the collision in moment space. Here $\mathbf{S} = \omega \mathbf{I}$ in the BGK model whereas ω on the diagonal of matrix $\mathbf{S}$ can be changed to a set of ω_i in the MRT model. And the relaxation matrix $\mathbf{S}$ in the MRT model is:

$$\mathbf{S} = \begin{pmatrix} \omega_0 & 0 & \dots & 0 \\ 0 & \omega_1 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \omega_{q-1} \end{pmatrix} \quad (3.44)$$

The moments, i.e. $\mathbf{m} = \mathbf{M} \mathbf{f}(\mathbf{x}, t)$, we mentioned above have to hold the conservation law of physical quantities. For example, the zeroth moment corresponds to the density, which requires $M_{0i} = 1$ as $m_0 = \rho = \sum f_i = \sum M_{0i} f_i$. The transformation matrix $\mathbf{M}$ consisting of orthogonal row vectors can be constructed through several ways like Hermite polynomials and Gram-Schmidt procedure⁶. The linear independence of row vectors guarantees the existence of $\mathbf{M}^{-1}$ and the independence of relaxation of each moment. In the MRT model, some relaxation parameters are related to physical quantities, shear and bulk viscosity, for example, and other relaxation parameters are not and can be,

⁶Details of procedure of construction is not presented and can be found in Krüger et al. [63]

therefore, freely chosen. Fine-tuning these freely chosen parameters can increase stability and accuracy, which is not guaranteed in the BGK model. However, the determination of an ideal set of relaxation parameters is time-consuming and empirical, as a universal parameter study has not existed.

TRT The two-relaxation-time (TRT) model is proposed to combine the algorithmic simplicity of the BGK model and the accuracy and stability advantage of the MRT model. With two relaxation rates ω_+ , related to kinematic viscosity, and ω_- , a free parameter, the accuracy and stability of the TRT model can be characterized by a so-called magic parameter:

$$\Lambda = \left(\frac{1}{\omega^+ \Delta t} - \frac{1}{2} \right) \left(\frac{1}{\omega^- \Delta t} - \frac{1}{2} \right) \quad (3.45)$$

Thus, the complexity of tuning relaxation parameters is dramatically decreased compared to the MRT model.

3.2.3 Chapman-Enskog analysis

As briefly mentioned in section 3.2.2, we have found the lattice Boltzmann equation, Equation(3.36), by discretizing the continuous Boltzmann equation and some relationships between discrete distribution function f and macroscopic values, i.e. $\sum f_i = \rho$ and $\sum f_i \mathbf{c}_i = \rho \mathbf{u}$. We still need to show the LBE itself can actually be employed to simulate the behavior of fluids, which is usually accomplished by solving the Navier-Stokes equation in conventional computational fluid dynamic(CFD) methods. Derivation of the Navier-Stokes equation from discrete LBE will be shown by the Chapman-Enskog analysis in this section. For simplicity, we ignore the external force and focus on the LBE with the BGK collision operator:

$$f_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) - f_i(\mathbf{x}, t) = -\frac{\Delta t}{\tau} (f_i(\mathbf{x}, t) - f_i^{\text{eq}}(\mathbf{x}, t)). \quad (3.46)$$

The Chapman-Enskog analysis is essentially a perturbation analysis for the particle distribution f_i . The Taylor expansion of f_i around the equilibrium distribution function f_i^{eq} with the Knudsen number K_n ⁷ as the expansion

⁷ K_n is a dimensionless number defined as the ratio of the molecular mean free path length to a representative physical length scale and small enough to serve as the expansion parameter

parameter. Here we use ϵ^n to indicate K_N^n . With the expansion, we can get $f = f^{(0)} + \epsilon f^{(1)} + \epsilon^2 f^{(2)} + \dots$, where $f^{(0)} = f^{eq}$, $\nabla f = \epsilon \nabla f^{(1)}$ for spatial gradient and the time derivative is $\partial_t f_i = \epsilon \partial_t^{(1)} f_i + \epsilon^2 \partial_t^{(2)} f_i + \dots$

By Taylor expanding the LBE, Equation(3.46), we get:

$$\Delta t (\partial_t + c_{i\alpha} \partial_\alpha) f_i + \frac{\Delta t^2}{2} (\partial_t + c_{i\alpha} \partial_\alpha)^2 f_i + O(\Delta t^3) = -\frac{\Delta t}{\tau} f_i^{neq} \quad (3.47)$$

where $f_i^{neq} = f_i - f_i^{eq}$. For finding the Navier-Stokes equation, we just need the two lowest orders so that the $O(\Delta t^3)$ and $O(\epsilon^3)$ term can be neglected. By multiplying $(\Delta t/2) (\partial_t + c_{i\alpha} \partial_\alpha)$ to both sides of the above equation, we can subtract the $(\partial_t + c_{i\alpha} \partial_\alpha)^2$ term and get:

$$\Delta t (\partial_t + \mathbf{c}_i \nabla) f_i + O(\Delta t^3) = -\frac{\Delta t}{\tau} f_i^{neq} + \Delta t (\partial_t + \mathbf{c}_i \nabla) \frac{\Delta t}{2\tau} f_i^{neq} \quad (3.48)$$

Applying the aforementioned perturbation of f and time and space derivatives and separating terms in the above equation to different orders, we can get the following equations:

$$\mathcal{O}(\epsilon) : f_i^{(0)} = f_i^{eq}(\mathbf{u}_f) \quad (3.49)$$

$$\mathcal{O}(\epsilon^1) : \Delta t (\partial_t^{(1)} + \mathbf{c}_i \nabla^{(1)}) f_i^{eq} = -\frac{\Delta t}{\tau} f_i^{(1)} \quad (3.50)$$

$$\mathcal{O}(\epsilon^2) : \Delta t (\partial_t^{(2)}) f_i^{eq} = -\frac{\Delta t}{\tau} f_i^{(2)} - \Delta t (\partial_t^{(1)} + \mathbf{c}_i \nabla^{(1)}) [1 - \frac{\Delta t}{2\tau}] f_i^{(1)} \quad (3.51)$$

The conservation of mass and momentum for the collision operator requires:

$$\sum_i f_i^{neq} = 0, \quad \sum_i \mathbf{c}_i f_i^{neq} = \mathbf{0}. \quad (3.52)$$

i.e.

$$\sum f_i^{(n)} = 0 \quad \text{and} \quad \sum \mathbf{c}_i f_i^{(n)} = \mathbf{0} \quad \text{for all } n \geq 1 \quad (3.53)$$

Taking the zeroth, first and second moment(i.e. multiplying by 1, $c_{i\alpha}$, $c_{i\alpha}c_{i\beta}$, respectively, and then summing over i) of Equation(3.50) and Equation(3.51) and combining the resulting equations, the macroscale mass and momentum

in continuum flow, which requires $K_n < 0.01$.

conservation can be found:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \quad (3.54)$$

$$\partial_t(\rho \mathbf{u}) + \nabla \cdot \Pi = 0 \quad (3.55)$$

where $\Pi = \sum_i c_{i\alpha} c_{i\beta} \left[f_i^{eq} + \left(1 - \frac{1}{2\tau}\right) f_i^{(1)} \right]$ is the momentum flux tensor. Taking the discretised form of f^{eq} :

$$f_i^{eq}(\mathbf{x}, t) = w_i \rho \left(1 + \frac{\mathbf{u} \cdot \mathbf{c}_i}{c_s^2} + \frac{(\mathbf{u} \cdot \mathbf{c}_i)^2}{2c_s^4} - \frac{\mathbf{u} \cdot \mathbf{u}}{2c_s^2} \right) \quad (3.56)$$

back to the flux tensor, we can get:

$$\Pi^{(0)} = \sum_i c_{i,\alpha} c_{i,\beta} f_i^{eq} = p \delta_{\alpha\beta} + \rho u_\alpha u_\beta \quad (3.57)$$

and

$$\Pi^{(1)} = \sum_i \left(1 - \frac{1}{2\tau} \right) f_i^{(1)} = \nu (\nabla_\alpha (\rho u_\beta) + \nabla_\beta (\rho u_\alpha)) \quad (3.58)$$

where $p = c_s^2 \rho$ and $\nu = (\tau - 1/2) c_s^2$ with $c_s = 1/\sqrt{3}$. Finally, the incompressible Navier–Stokes equation is recovered:

$$\partial_t(\rho \mathbf{u}) + (\mathbf{u} \cdot \nabla)(\rho \mathbf{u}) = -\nabla p + \nu \nabla^2(\rho \mathbf{u}) \quad (3.59)$$

3.2.4 Boundary conditions

In traditional computational fluid dynamics methods (CFD), such as finite element methods (FEM) or finite volume methods (FVM), appropriate descriptions of boundary condition and initial condition⁸ are of great importance for constructing a complete set of partial differential equations (PDEs), i.e. Navier-Stokes equations (NSE). In the LBM, the importance should not be underestimated as well. However, there are no unique and direct links between

⁸The initial state in our simulations is usually set to equilibrium, i.e. $f_i(\mathbf{x}, t = 0) = f_i^{eq}(\rho(\mathbf{x}, t = 0), \mathbf{u}(\mathbf{x}, t = 0))$ as the statistical long-time behaviour of suspension systems is usually independent of the initial state. For non-homogeneous initial conditions, the initialization usually contains two components: $f_i(\mathbf{x}, t = 0) = f_i^{eq}(\mathbf{x}, t = 0) + f_i^{neq}(\mathbf{x}, t = 0)$. The non-equilibrium part is determined by specific physical problems and not included in our discussion.

macroscopic boundary conditions, such as Dirichlet (no-slip) and Neumann (free-slip) boundary conditions straightforwardly imposed in traditional CFD, and particle distribution function f_i on the mesoscale. In other words, one “expression” of particle distribution function f_i corresponds to one macroscopic boundary condition, whereas the inverse operation is not unique. Therefore, boundary conditions for the LBM are somewhat more complex, and countless boundary conditions have been proposed. Here we group boundary conditions into two categories: with or without a wall, and mainly discuss periodic boundary conditions (PBCs), including Lees-Edwards boundary condition (LEbc) and the standard bounce-back (SBB), the most widely used and simplest to implement wall boundary condition in the LBM. In this section, we focus on 2D applications and use D2Q9 velocity sets, as shown in Figure3.4(A), for illustration.

Periodic boundary condition

Periodic boundary conditions (PBCs) are a set of boundary conditions which use a small part called a unit cell for approximating a large (infinite) system and are frequently employed in numerical simulations and mathematical models for reducing computational time. The implementation of standard periodic conditions in the LBM is quite straightforward. The distribution functions f_i^* , inside the domain but not close to the boundary read as:

$$f_i^*(\mathbf{x}, t) = f_i^*(\mathbf{x} + \mathbf{L}, t) \quad (3.60)$$

where f_i^* denotes the particle distribution function after collision. $\mathbf{L}$ has the direction the same as the periodic direction and the length of the simulation box in the periodic direction.

For dealing with lattices close to the inlet and outlet boundaries, we include “virtual” lattices for implementation. As shown in Figure3.5, lattice nodes close to the boundaries are located in x_1 and x_N with a distance $0.5\Delta x$ to the periodic boundaries with coordination x_{inlet} and x_{outlet} in the x -direction. The periodicity length is given by $L = x_{out} - x_{in} = (x_N + 0.5\Delta x) - (x_1 - 0.5\Delta x) = x_N - x_1 + \Delta x = N\Delta x$. The “virtual” lattices are added before and after the periodic boundaries, represented by dashed circles, with a distance $0.5\Delta x$. Before the streaming step, the particle distribution functions f_i^* are copied to these “virtual” lattices from

the opposite periodic boundaries:

$$\begin{aligned}
 f_i^*(x, t) = f_i^*(x + L, t) &\implies \begin{cases} f_1^*(x_0, y_2, t) = f_1^*(x_N, y_2, t) \\ f_5^*(x_0, y_2, t) = f_5^*(x_N, y_2, t), \\ f_8^*(x_0, y_2, t) = f_8^*(x_N, y_2, t) \end{cases} \\
 f_{-i}^*(x + L, t) = f_{-i}^*(x, t) &\implies \begin{cases} f_3^*(x_{N+1}, y_2, t) = f_3^*(x_1, y_2, t) \\ f_6^*(x_{N+1}, y_2, t) = f_6^*(x_1, y_2, t). \\ f_7^*(x_{N+1}, y_2, t) = f_7^*(x_1, y_2, t) \end{cases}
 \end{aligned} \tag{3.61}$$

Here $-i$ denotes the opposite direction of i .

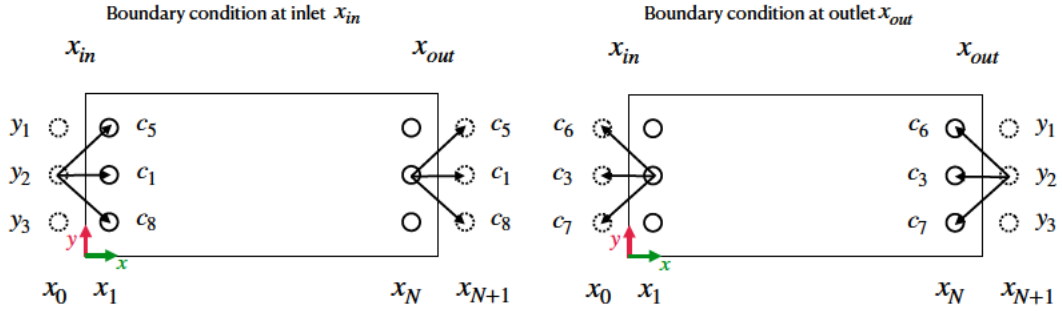


Figure 3.5 Sketch of the periodic boundary condition in LBM. Layers of “virtual” nodes, denoted by dashed circles, are added before and after the periodic boundaries, i.e. at $x_0 = x_1 - \Delta x$ and $x_{N+1} = x_N + \Delta x$, respectively. Figure is adapted from Krüger et al. [63].

Despite the standard periodic boundary conditions, there are flow problems with a periodic velocity field but non-periodic pressure or density field, such as pressure-driven flow in the channel. Kim and Pitsch [59] proposed a generalized periodic boundary condition for simulating a pressure-driven flow in a periodic geometry based on the algorithms by Zhang and Kwok [139]. Details of this kind of periodic boundary will be introduced in Chapter 6 as it is related to our channel flow simulation.

Lees-Edwards boundary condition

The Lees-Edwards boundary conditions (LEbc) are an extension of standard periodic boundary conditions, originally developed by Lees and Edwards [76] for molecular dynamics simulations of a simple shear flow. LEbc are quite popular in research of rheology as they removes the wall effect and is introduced to the LBM by Wagner and Pagonabarraga [132]. In molecular dynamics or discrete

element method (DEM), the basic algorithms of LEbc read as:

$$\begin{aligned}
r'_x &= \begin{cases} (r_x + d_x) \bmod L_x & r_y \geq L_y \\ r_x \bmod L_x & 0 \leq r_y < L_y \\ (r_x - d_x) \bmod L_x & r_y < 0 \end{cases} \\
r'_y &= (r_y \bmod L_y) \\
r'_z &= (r_z \bmod L_z) \\
v'_x &= \begin{cases} v_x + U_x & r_y \geq L_y \\ v_x & 0 \leq r_y < L_y \\ v_x - U_x & r_y < 0 \end{cases} \\
v'_y &= v_y \\
v'_z &= v_z
\end{aligned} \tag{3.62}$$

where $d_x = tU_x$ and “mod” is short for “modulo” or “modulus”. As shown in Figure3.6(A), the shear rate is $\dot{\gamma} = U_x/L_y$.

For implementing the LEbc in the LBM, two modifications should be added to the particle distribution function f_i when crossing the system boundaries in the velocity gradient direction, i.e. y-direction in Figure3.6. The first modification is a Galilean transformation, reading as :

$$f_i^G(\mathbf{x}, t) = f_i(\mathbf{x}, t) + f_i^{eq}(\mathbf{x}, \mathbf{u} + \mathbf{U}_{shear}) - f_i^{eq}(\mathbf{x}, \mathbf{u}, t) \tag{3.63}$$

where $\mathbf{U}_{shear}$ is the shear velocity, and the shear rate is $\dot{\gamma} = \mathbf{U}_{shear}/L_y$.

Second is the shift in position⁹:

$$f_i(x + dI, t) = (1 - dR)f'_i(x, t) + dRf'_i(x - 1, t) \tag{3.64}$$

where the shifted distance $d = tU_x$ is split into an integer part dI and real part dR with $0 \leq dR \leq 1$ as the resulting shifted position does not necessarily correspond to an integer multiple of the lattice spacing.

⁹Here we only consider about the shear direction (x-direction).

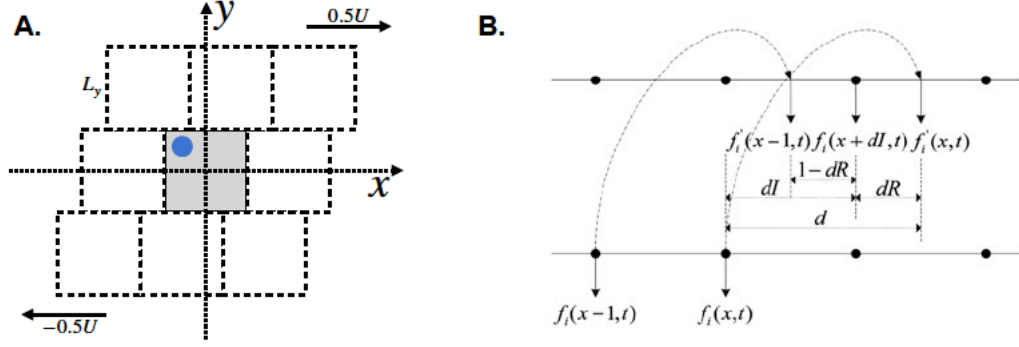


Figure 3.6 (A) The periodic domain images of Lees-Edwards boundary condition. The upper plane moves with a constant velocity of $0.5U$, and the lower plane moves with $-0.5U$. The shear rate is $\dot{\gamma} = U/L_y$. (B) Illustration of the outgoing f_i leaving the lower boundary and entering the upper boundary. $d = tU$ is the position shift going across the Lees-Edwards boundary. Figure(B) is adapted from Zhou et al. [141]

Wall boundary conditions

Boundary conditions for walls can be basically grouped into two categories according to the location of the boundary nodes, as shown in Figure 3.7: the link-wise type where the boundary lies in the middle of fluid and solid nodes and wet-node type where the boundary lies on solid nodes.

Link-wise In link-wise schemes, the standard bounce back (SBB) method, [67][44][33][142] is the old but most popular wall boundary condition in the LBM due to its simplicity for implementation. The principle of the SBB is that particle distribution functions f_i coming from the fluid and hitting the wall during the streaming step are reflected back to where they originally came from. The principle of the SBB ensures a **no-slip** boundary condition, also known as the Dirichlet boundary condition with no tangential velocity, can be implemented in the LBM.

For rest walls, the principle can be implemented as follows:

$$f_i(\mathbf{x}, t + \Delta t) = f_i^*(\mathbf{x}, t) \quad (3.65)$$

For the case shown in Figure 3.7, the implementation is:

$$\begin{aligned} f_2(x, t + \Delta t) &= f_4^*(x, t), \\ f_5(x, t + \Delta t) &= f_7^*(x, t), \\ f_6(x, t + \Delta t) &= f_8^*(x, t). \end{aligned} \quad (3.66)$$

The standard bounce-back formula for a moving wall reads:

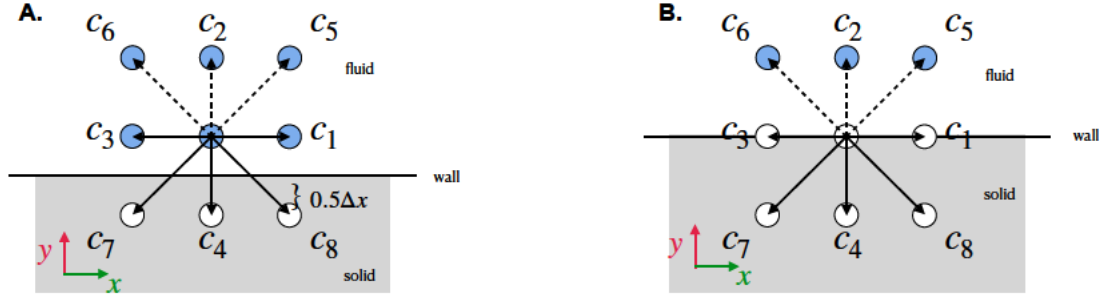


Figure 3.7 Sketch of link-wise and wet-node boundary conditions. Fluid nodes and solid nodes are represented by blue circles and open circles, respectively. (A). Link-wise: wall boundary is located in the middle of fluid nodes and solid nodes. (B). Wet-node: wall boundary is located on solid nodes. At time t , particle distribution functions f_i , denoted as c_i experience a collision step to f_i^* . Unknown distribution functions after propagation, i.e. at time $t + \Delta t$, are represented by dashed vectors.

$$f_{-i}(x, t + \Delta t) = f_i^*(x, t) - 2w_i \rho u_b \cdot c_i \quad (3.67)$$

where u_b is the velocity of the wall boundary.

Wet-node In wet-node schemes, boundaries are located on lattice nodes, as shown in Figure 3.7, which means the continuity of fluid should be satisfied at the boundary. Thus macroscopic quantities like density or velocity have to be incorporated in constructing boundary conditions in the LBM. Here we briefly mention a popular strategy called the non-equilibrium bounce-back method (NEBB) or Zou-He method proposed by He et al. [44], and this is what we are using in our simulation.

As suggested by its name, the working principle of NEBB is providing values for the unknown particle distribution functions, represented by dashed vectors in Figure 3.7(B) by applying the bounce-back rule for their non-equilibrium part:

$f_{-i}^{neq}(\mathbf{x}_b, t) = f_i^{neq}(\mathbf{x}_b, t)$, where $\mathbf{x}_b$ denotes lattices on the boundary. Combining with requirements arising from the continuity of macroscopic density or velocity, which are evaluated locally by $\rho = \sum_i f_i$ and $\rho \mathbf{u} = \sum f_i \mathbf{c}_i$, the unknown distribution functions can be determined. The NEBB method makes full use of all already available information, which improves its accuracy[73] but also improves its complexity for implementation in 3D. There are many other wet-node boundary conditions developed. For example, Skordos [122] take fluid velocity gradient into consideration for increasing the accuracy, and Inamuro et al. [49] replaces the unknown populations by an equilibrium function to impose the correct wall velocity. Latt et al. [73] conducted a comparison between five commonly adopted wet-node, also called on lattice, approaches, aforementioned ones are included, and found that there is no generally advised optimal boundary choice as the choice depends on the simulation geometry and on a competing influence between stability and accuracy.

3.3 LB-DEM coupling

Various approaches have been proposed for coupling the fluid phase and the solid phase. Here we will concisely talk about three different approaches: the bounce-back method (BB), immersed boundary method (IBM) and the partially saturated cell method (PSM).

3.3.1 Bounce back method

As discussed above, bounce-back is the most widely used no-slip boundary condition for the LBM because of its locality, simplicity and efficiency. The most straightforward way for applying a bounce-back scheme in fluid-solid coupling is to approximate a curved boundary of solid objects, which are solid spheres in our simulations, by a staircase, as shown in Figure 3.8. This coupling approach was proposed by Ladd [67] and named a simple bounce-back (SBB) method. With a staircase approximation, lattice nodes can be divided into four categories and indicated by different colours in Figure 3.8 : (1). exterior fluid nodes (white) - a fluid node not connected to any solid node; (2). interior solid node (blue) - a solid node not connected to any fluid node; (3). fluid boundary node (green) - a fluid node connected to at least one solid node; (4). solid boundary node (yellow)

- a solid node connected to at least one fluid node. Here, fluid and solid nodes are located outside and inside the particle boundary, respectively. A link between a fluid boundary node and a solid boundary node is called a boundary link. It is obvious that the staircase approximation results in geometrical discretisation error, especially for particles that are relatively small compared to the lattice size, i.e. $d_p/\Delta x \sim \mathcal{O}(1)$. However, the simplicity and ease of implementation of SBB can not be overlooked, which makes SBB still very popular.

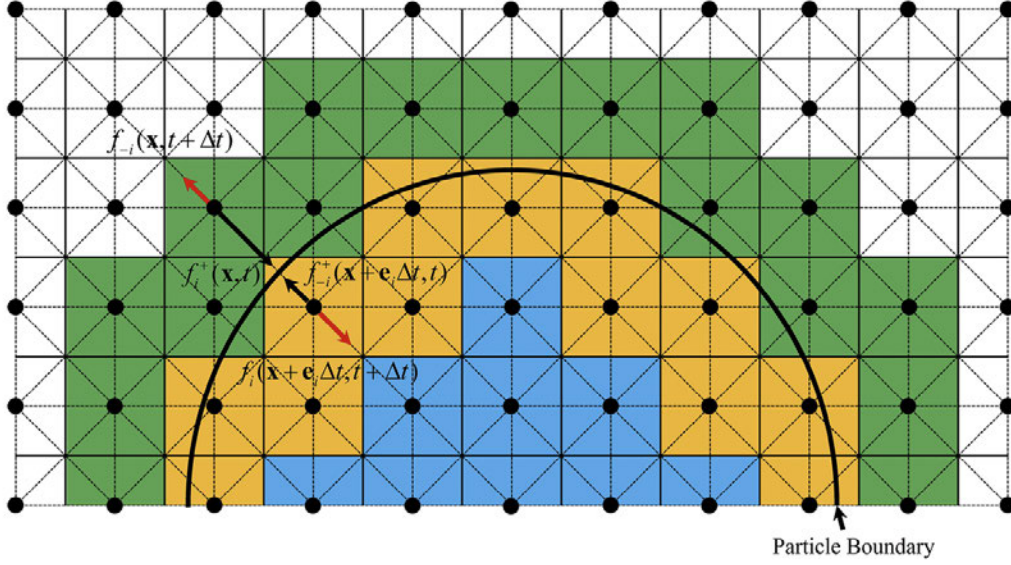


Figure 3.8 Sketch of bounce back method, taken from Liu and Wu [80]

For rigid moving particles, the velocity of the particle boundary is given by:

$$\mathbf{u}_b = \mathbf{u}_p + \boldsymbol{\Omega}_p \times \left(\mathbf{x} + \frac{1}{2} \mathbf{c}_i - \mathbf{x}_{p,c} \right) \quad (3.68)$$

where $\mathbf{u}_p$, $\boldsymbol{\Omega}_p$, $\mathbf{x}_{p,c}$ are the translation velocity, angular particle velocity and center of the solid particle, respectively. The bounce-back procedure, based on local momentum transfer between distribution functions of fluid boundary nodes and solid boundary nodes, denoted as arrows in Figure 3.8, can be calculated by:

$$\begin{aligned} f_{-i}(\mathbf{x}, t + \Delta t) &= f_i^*(\mathbf{x}, t) - 2w_i \rho \mathbf{u}_b \cdot \mathbf{c}_i \\ f_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) &= f_{-i}^*(\mathbf{x} + \mathbf{c}_i \Delta t, t) + 2w_i \rho \mathbf{u}_b \cdot \mathbf{c}_i \end{aligned} \quad (3.69)$$

Hence, the local force on the boundary nodes can be calculated through a

momentum exchange at the boundary links, reading:

$$\begin{aligned} \mathbf{F}_{LBM,node} \left(\mathbf{x} + \frac{1}{2} \mathbf{c}_i \Delta t, t + \frac{1}{2} \Delta t \right) = & 2 \left[f_i^+(\mathbf{x}, t) - f_{-i}^+(\mathbf{x} + \mathbf{c}_i \Delta t, t) \right. \\ & \left. - 2\omega_i \rho \mathbf{u}_b \cdot \mathbf{c}_i \right] \cdot \mathbf{c}_i. \end{aligned} \quad (3.70)$$

The total hydrodynamic force and the torque acting on the particle are then calculated by summing over all the boundary links:

$$\begin{aligned} \mathbf{F}_H &= \sum_i \mathbf{F}_{LBM,node}, \\ \mathbf{M}_H &= \sum_i \left(\mathbf{x} + \frac{1}{2} \mathbf{e}_i \Delta t - \mathbf{X}_p \right) \times \mathbf{F}_{LBM,node}. \end{aligned} \quad (3.71)$$

From the equations above, we can find that roles played by fluid nodes and solid bodies are equivalent in the coupling procedure, which is counterintuitive. At high Reynolds numbers, the rigidity of particles will be influenced if nodes inside particles have the same dynamics as the fluid. Therefore, Ladd's method is limited to particles having a much larger density than the fluid and Aidun et al. [3] proposed an alternative method which removes the fluid nodes within particles to overcome the limitation of SBB, whereas the mass conservation is broken under Aidun's method. Hence, some modified versions of the momentum exchange [19][81] have been proposed to improve Galilean invariance.

For precisely describing the curved boundaries with higher accuracy than SBB, the interpolated bounce-back (IBB) method was proposed by Bouzidi et al. [10]. As the name suggested, the basic idea of IBB is to include a spatial interpolation with a weighting parameter q for determining the exact location of the fluid-solid interface during the bounce-back process, which is proven to maintain second-order accuracy. Here, we denote the locations of a solid boundary node and a fluid boundary node, which form a boundary link, as $\mathbf{x}_s$ and $\mathbf{x}_f$, respectively. Moreover, the intersection of this boundary link with the particle boundary is denoted as $\mathbf{x}_b$. Thus, the weighting parameter q measures the relative location of the particle boundary in the boundary link and is given by:

$$q = |\mathbf{x}_f - \mathbf{x}_b| / |\mathbf{x}_f - \mathbf{x}_s| \quad (3.72)$$

With the weight parameter q , there are several interpolation strategies proposed, such as a linear interpolation and a quadratic interpolation by Bouzidi et al. [10]

and a double interpolation by Yu et al. [137] for improving the SBB accuracy in describing complex geometries. Due to the locality, simplicity and efficiency of the bounce-back method, SBB and its extension IBB are quite popular for coupling of the fluid and solid phases and widely used in the simulations of suspensions. For example, a simple shear between two sheared walls by Kulkarni and Morris [64], Haddadi and Morris [42] and a simple shear with LEbc by Lorenz et al. [81] with a correction for LEbc based on Aidun et al. [3]. However, they also have some limitations for specific cases. For example, one disadvantage of the IBB is the requirement of extra fluid nodes between particles [56], which means the discontinuity of physical quantities might occur when simulating suspensions or porous media with very high solid volume fractions, where the gap distances between solid particles could be very small. Another disadvantage of the bounce-back method is mass conservation, as mentioned before, which is important for simulating deformable particles such as blood cells and polymers.

3.3.2 Immersed boundary method

The immersed boundary method (IBM), proposed by Peskin [105] to simulate fluid-structure interactions in computational fluid dynamics (CFD), is a classical method older than the LBM. With its simplicity in the implementation of complex boundaries, IBM was introduced into the LBM by Feng and Michaelides [29]. The combination of the IBM and the LBM is also called the immersed-boundary-lattice-Boltzmann method (IB-LBM).

The basic idea of the IB-LBM is to introduce a set of Lagrangian meshes, capturing the boundary of solid objects, that moves relative to the fluid, meshed by Eulerian lattices in the LBM. Coupling between the solid phase, described by Lagrangian meshes, and the fluid phase, meshed by Eulerian lattices, is accomplished through the velocity interpolation (Eulerian to Lagrangian) and force spreading (Lagrangian to Eulerian) steps, as shown in Figure 3.9. Here subscripts s and f represent the solid and fluid phases, respectively.

The velocity interpolation and force spreading are calculated through discretised IBM equations, which read:

$$\mathbf{u}_s(\mathbf{x}_s, t) = \sum_f \Delta x^3 \mathbf{u}_f(\mathbf{x}_f, t) D(\mathbf{x}_f - \mathbf{x}_s) \quad (3.73)$$

$$\mathbf{F}_f(\mathbf{x}_f, t) = \sum_s \mathbf{F}_s(\mathbf{x}_s, t) D(\mathbf{x}_f - \mathbf{x}_s) \Delta A \quad (3.74)$$

where ΔA is the control length occupied by the boundary point¹⁰ and $D(x)$ is the kernel function:

$$D(\mathbf{x}_f - \mathbf{x}_s) = \frac{1}{\Delta x^r} \delta\left(\frac{x_f - x_s}{\Delta x}\right) \delta\left(\frac{y_f - y_s}{\Delta x}\right) \delta\left(\frac{z_f - z_s}{\Delta x}\right) \quad (3.75)$$

and

$$\delta(r) = \begin{cases} \frac{1}{4} \left(1 + \cos\left(\frac{\pi|r|}{2}\right)\right) & , |r| \leq 2 \\ 0, & |r| > 2 \end{cases} \quad (3.76)$$

The idea of such transformation is similar to coarse-graining, i.e. the physical quantity $\mathbf{\Pi}$ at point $\mathbf{X}$ is contributed by its surrounding points multiplying a weighting function, which is related to the distance between two points.

The force acted on the solid boundary from the fluid-solid interaction can be calculated from the following equation:

$$\mathbf{F}_s(\mathbf{x}, t) = \rho_f (\mathbf{U}_s(\mathbf{x}, t) - \mathbf{u}_s(\mathbf{x}, t)) / \delta t, \quad (3.77)$$

where $\mathbf{U}_s$ is the actual velocity of the Lagrangian points and $\mathbf{u}_s$ is the velocity calculated from Equation(3.73) in the IBM algorithm. The force is generated from the change of the momentum divided by the collision time δt , derived by Wu and Aidun [134]. There are other approaches proposed to model rigid bodies in IBM, such as that of Lai and Peskin [69].

Considering the force spread from Lagrangian meshes, the lattice Boltzmann equation (LBE) reads:

$$f_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) = f_i(\mathbf{x}, t) + \Omega_i^f \Delta t + F_i^{external} \Delta t + F_i^{couple} \Delta t \quad (3.78)$$

where $F_i^{external}$ describes the external force like gravity, which is similar to and F_i^{couple} represents force from Lagrangian meshed. The formula of discrete force distribution F_i^{couple} is proposed by Guo et al. [38]:

$$\mathbf{F}_i^{couple}(\mathbf{x}, t) = \left(1 - \frac{1}{2\tau}\right) \omega_i \left[3 \frac{\mathbf{c}_i - \mathbf{u}(\mathbf{x}, t)}{c^2} + 9 \frac{\mathbf{c}_i \cdot \mathbf{u}(\mathbf{x}, t)}{c^4} \mathbf{c}_i \right] \cdot \mathbf{F}_f(\mathbf{x}, t) \quad (3.79)$$

where $\mathbf{F}_f$ is the force density at Eulerian meshes of fluid, as shown in Figure 3.9.

¹⁰ ΔA will be the surface area in 3D case

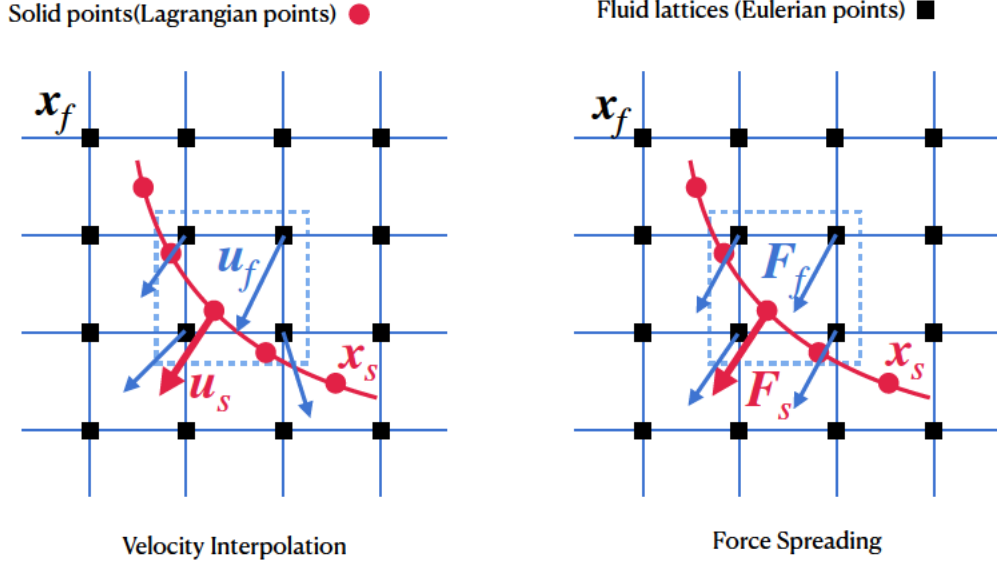


Figure 3.9 An illustration of how the fluid and solid phase coupled in IB-LBM. Red points on the boundary of the immersed object are Lagrangian points, and black points on the meshed grids are Eulerian lattices of the fluid phase. Left: particle velocity $u_s(x_s, t)$ (red arrow on Lagrangian points) is interpolated from the surrounding fluid velocities $u_f(x_f, t)$ of Eulerian lattices (blue arrows). Right: force on each particle $F_s(x_s, t)$ (red arrow on Lagrangian points) is spread out to the fluid lattices $F_f(x_f, t)$ (blue arrows on Eulerian lattices). Figure is adapted from Tan et al. [127].

The general algorithm for an IB-LBM coupling consists of the following steps:

1. Perform the propagation/streaming step of the LB algorithm and calculate the uncorrected velocity from the relationship: $\mathbf{u}_f = \frac{\sum f_i \mathbf{c}_i}{\rho}$.
2. Velocity interpolation: use Equation(3.73) and the kernel equation(Equation(3.75)) to interpolate the velocity of Lagrangian points $\mathbf{u}_s$.
3. Calculate the force $\mathbf{F}_s$ acted on the boundary points using Equation(3.77).
4. Force spreading: use Equation(3.74) to calculate the force density $\mathbf{F}_f$ at each Eulerian lattice.
5. The velocity of each Eulerian lattice is updated by:

$$\mathbf{U}_f(\mathbf{x}) = \mathbf{u}_f(\mathbf{x}) + \frac{\mathbf{F}_f(\mathbf{x})\Delta t}{2\rho} \quad (3.80)$$

6. Perform the collision step with corrected velocity $\mathbf{U}_f$ and force density $\mathbf{F}_f$ by using Equation(3.78) and Equation(3.79).
7. Go back to Step 1.

With Lagrangian meshed introduced, the IBM has a major advantage over other boundary conditions in simulating deformable objects, such as polymers and biological cells Schiller et al. [113] and elastic properties, such as dilation, shear and bending resistance Tan et al. [127], whereas the advantage will turn to disadvantage because of the inefficiency for implementing the IBM and the computational complexity, especially when the Eulerian lattice is large.

3.3.3 Partially saturated cell method

The partially saturated cell methods, proposed by Noble and Torczynski [99], provide a kind of weighting strategy to include the existence of the solid phase, which can be seen as a hybrid of standard LBM bounce-back methods and immersed-boundary methods. In this method, the lattice Boltzmann equation is modified to include an additional collision term, which depends on the local volume fraction of the solid in the given lattice cell,

$$f_i(\mathbf{x} + \Delta t \mathbf{c}_i, t + \Delta t) = f_i(\mathbf{x}, t) + [1 - B(\mathbf{x}, \tau)]\Omega_i^f + B(\mathbf{x}, \tau)\Omega_i^s \quad (3.81)$$

where $\Omega_i^f = \frac{\Delta t}{\tau} f_i(\mathbf{x}, t) - f_i^{eq}(\mathbf{x}, t)$ for BGK collision operator and $B(\mathbf{x}, \tau)$ is a weighting function related to the solid fraction ϵ_s of the lattice node at $\mathbf{x}$. Noble and Torczynski [99] suggested two kinds of collision models Ω_i^s for the solid phase. The first and most popular one is inspired by the non-equilibrium bounce-back boundary condition:

$$\Omega_i^s = f_{-i}(\mathbf{x}, t) - f_i(\mathbf{x}, t) + f_i^{eq}(\rho, \mathbf{U}_s) - f_{-i}^{eq}(\rho, \mathbf{u}) \quad (3.82)$$

where $\mathbf{U}_s$ is the particle velocity and $\mathbf{u}$ is the fluid velocity. Both of these two velocities are individually considered on each lattice node. The second suggestion, called the superposition method, is:

$$\Omega_i^s = f_i^{eq}(\rho, \mathbf{U}_s) - f_i(\mathbf{x}, t) \left(1 - \frac{\Delta t}{\tau} (f_i(\mathbf{x}, t) - f_i^{eq}(\rho, \mathbf{u}))\right) \quad (3.83)$$

Holdych [47] suggested a minor modification of the solid collision term in Equation(3.82) by substituting the fluid velocity by the particle velocity:

$$\Omega_i^s = f_{-i}(\mathbf{x}, t) - f_i(\mathbf{x}, t) + f_i^{eq}(\rho, \mathbf{U}_s) - f_{-i}^{eq}(\rho, \mathbf{U}_s) \quad (3.84)$$

The weighting function $B(\mathbf{x}, \tau)$ has different forms. Noble and Torczynski [99] proposed a linear weighting function of the lattice solid fraction,

$$B(\mathbf{x}, \tau) = \epsilon_s \quad (3.85)$$

and a non-linear form:

$$B(\mathbf{x}, \tau) = \frac{\epsilon_s(\tau/\Delta t - 1/2)}{(1 + \epsilon_s) + (\tau/\Delta t - 1/2)} \quad (3.86)$$

where ϵ_s denotes the solid fraction on the lattice nodes, which has to be accurately determined.

Hydrodynamic force and torque The hydrodynamic force and torque acting on a particle can be computed by summing the product of Ω_i^s with the solid fraction weighting function B overall solid covered lattice nodes with a lattice

spacing of h in d dimensions:

$$\begin{aligned}\mathbf{F}^H &= \frac{h^d}{\Delta t} \sum_n B_n \sum_i \Omega_i^s \mathbf{c}_i \\ \mathbf{T}^H &= \frac{h^d}{\Delta t} \sum_n (\mathbf{x} - \mathbf{x}_s) \times \left(B_n \sum_i \Omega_i^s \mathbf{c}_i \right) = \sum_n (\mathbf{x} - \mathbf{x}_s) \times \mathbf{F}^H.\end{aligned}\tag{3.87}$$

The update of ϵ_s for moving boundaries is the most challenging part of the PSM. Thus, many different methods have been proposed for the calculation of ϵ_s , such as exact closed-form, i.e. analytical, solution, sub-cell method, polygonal approximation[16], Monte-Carlo approximation, linear approximation and so on[54][104]. Here we briefly mention the sub-grid method and what we are using in our simulations. As shown in Figure3.10(b), the lattice cell is decomposed into smaller cells, here we call these smaller cells as subgrids, and the number of subgrids inside the particle, $N_{grid,particle}$, are used to compute the solid fraction $\epsilon_s = N_{grid,particle}/N_{grid/lattice}$. This method is universally applicable and straightforward for implementation, but the computational cost will dramatically increase for finer resolution. Figure3.11 shows the results calculated with the sub-cell method. According to Najuch [94], setting the subgrid resolution to be 10, i.e. $L_{lattice} = 10 * L_{subgrid}$, gives a good trade-off between accuracy and computational cost in our LBDEM simulations.

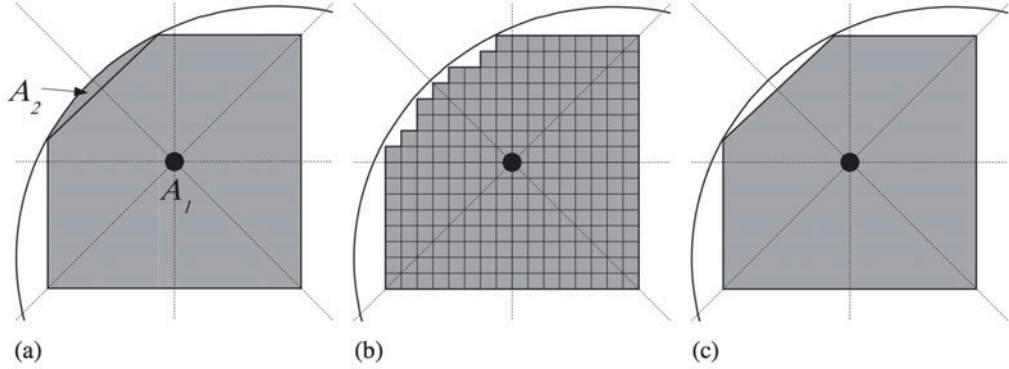


Figure 3.10 Sketches of three different methods for calculating solid fraction on the lattice nodes ϵ_s in 2D. (a). an exact closed-form solution, (b). sub-cell method, (c). polygonal approximation. Figure is taken from Owen et al. [104]

Although the sub-cell method for calculating ϵ_s will increase the computational cost, the implementation of the PSM with the sub-cell method is quite straight-

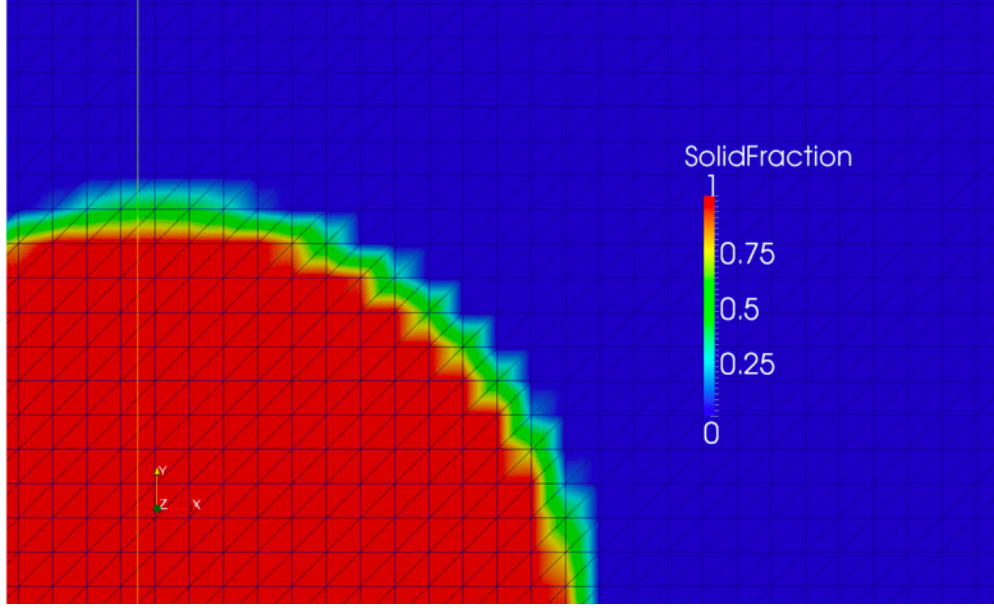


Figure 3.11 Snapshot of solid fractions ϵ_s results from Paraview. Different colours mean different values of solid fractions. Here ϵ_s is calculated through the sub-cell method from our LBDEM simulations.

forward, and no additional data storage or re-organisation of lattices is needed once lattices and subgrids are meshed, which is an advantage over other coupling methods. Besides, unlike the SBB and IBB, the PSM conserves the mass exactly and does not require the treatment of fresh fluid nodes. Unlike the IBB, which requires extra fluid nodes between particles, PSM only focuses on the solid fraction on each lattice. These advantages make the PSM a promising candidate for dense suspensions[82] and porous media with small pore sizes.

According to the brief discussion about three different methods for fluid-solid coupling, PSM is our choice for simulations of dense suspension with DEM and a coupled LBM. Furthermore, analytical and numerical comparisons between the non-equilibrium bounce back in Equation(3.84) and the superposition models Equation(3.83) in their capability of accurately computing the hydrodynamic stresslet was conducted, and the SP method was recommended in the PSM-LBDEM simulations of suspensions by Najuch and Sun [93].

3.3.4 Lubrication correction

The fluid flow can be resolved by fluid-solid coupling approaches, whereas the resolution of LBM, i.e. lattice size, is limited because of the computational

expenses. Thus, the fluid flow cannot be precisely resolved when particles are in close contact, and the gap distance between particles is smaller than the lattice size, which is inevitable in dense suspensions. As discussed in section 3.1.3, the

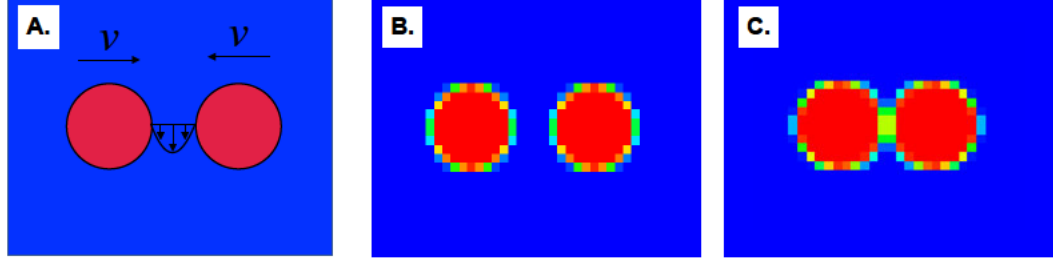


Figure 3.12 Sketches of lubrication force in three different cases. Two particles are moving towards each other with fixed velocity v in these three cases. (A). Lubrication force is analytically calculated with Equation(3.15). (B). Lubrication force is calculated from simulation, and the gap distance between particles is larger than one lattice size. (C). Lubrication force is calculated from simulation, and the gap distance between particles is smaller than one lattice size. Here the lattice size is $1/10$ of particle diameter, i.e. $L_{lattice} = 1/10d_p$. Different colours in figure (B) and (C) means different solid fractions calculated from the partially saturated cell method(PSM). Red and blue correspond to solid and fluid, respectively.

As shown in Figure 3.12, two particles immersed in the fluid are moving towards each other, and the lubrication force arises when particles are close to each other. In Figure 3.12(A), the lubrication force can be precisely calculated according to Equation(3.15). In Figure 3.12(B), the lubrication force can be simulated by LBDEM when the gap distance is larger than the lattice size. The lattice size shown in this figure is $L_{lattice} = 0.1d_p$. In Figure 3.12(C), the lubrication force cannot be precisely simulated as the gap distance is smaller than the lattice size. Related results can also be found in Figure 3.13 where analytical results and simulation results match very well when the dimensionless gap distance $\xi = \Delta x/d_p$ is larger than 0.1, which is the size ratio between lattice size and particle size. When $\xi = \Delta x/d_p$ is smaller than 0.1, the force acting on the particle

calculated from LBM¹¹ can not capture the divergence of the lubrication force. To recover the accuracy of the lubrication force in LBDEM simulations, we have implemented a modified lubrication force that combines the analytical and LBM-based forces into the DEM part. Based on the numerical and analytical results of lubrication force, the modified lubrication correction, based on [98], can be expressed as:

$$\mathbf{F}_{\alpha, \text{correction}}(\beta, \xi) = \mathbf{F}_{\alpha}(\beta, \xi) - \mathbf{F}_{\alpha}(\beta, \delta_{\text{cut}} \xi_N), \text{ for } \xi \leq \delta_{\text{cut}} \xi_N = \delta_{\text{cut}} h_{\text{lattice}} \quad (3.88)$$

where $\beta = d_i/d_j$ is the particle size ratio, $\xi = \Delta x/d_p$ is the dimensionless gap distance and δ_{cut} is a cut-off calibration parameter for the lubrication force correction. We can find that the lubrication correction, indicated by the black line in Figure 3.13, can serve as a solution for a precise calculation of lubrication force in LBDEM simulations once the cut-off parameter δ_{cut} is carefully calibrated. For tangential and rotational contributions, similar calibrations have also been done by Najuch [94] and related parameters such as relaxation parameter τ , lattice size L_{lattice} and cut-off parameters δ_{cut} for normal, tangential, rotational components will be used in our simulations. Lorenz et al. [82] also proposed a modified lubrication correction so that corrected values of lubrication forces as well as their first derivative, are continuous functions of the gap distances. Both the lubrication force mentioned in Section 3.1.3 and the lubrication force modification discussed here are approximations that apply to pairwise cases. It is extremely difficult to analytically solve for the accurate lubrication force when many particles gather together. As a result, the sum of pairwise lubrication forces can only provide a rough approximation. However, despite these limitations, incorporating lubrication forces into LBDEM simulations is necessary for accurately capturing the behavior of dense suspension systems.

Simulation procedure for LB-DEM coupling According to the discussion above, we can summarise our simulation methodology for simulating dense suspensions with LB-DEM coupling:

- Discrete element method (DEM), open-source software LAMMPS[128] and LIGGGHTS[60], to track particles:

$$m_i \ddot{\mathbf{x}}_i = \mathbf{F}_{\text{coll},i} + \mathbf{F}_{\text{hydrodynamic},i} + \mathbf{F}_{\text{lubrication}(-\text{correction}),i} + \mathbf{F}_{\text{others},i}$$

¹¹When the gap distance is very small, LBM can still calculate a lubrication force based on the surrounding fluid field as shown in Figure 3.12(C)

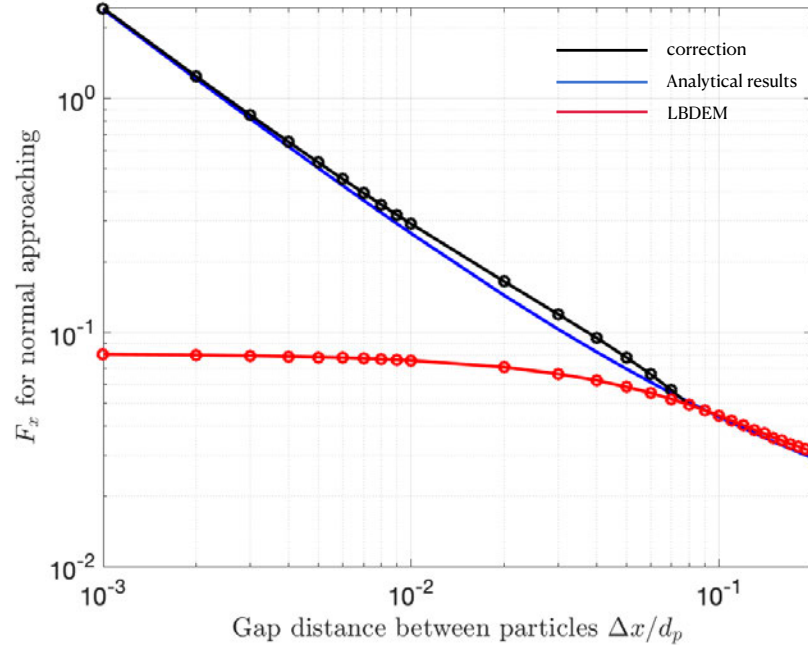


Figure 3.13 Lubrication forces as a function of gap distance between particles for two particles approaching each other in the normal direction. Redline is calculated from our LBDEM simulation with $L_{lattice} = 1/10d_p$ and blue line is analytical results calculated from Equation(3.15). The black line is the lubrication force after correction.

where $\mathbf{F}_{others,i}$ contains interactions such as electrostatic interaction, Brownian motion and van der Waals, which can be implemented into LAMMPS and LIGGGHTS.

- Lattice Boltzmann method (LBM), open-source software [74], to compute fluid flow
- Fluid-solid coupling through partially saturated cell method (PSM), contributed by Najuch [94] and Seil [115], for calculating hydrodynamic force on particles
- Necessary information for LBM: Particle velocity and position (+ shape for non-spherical particle)

Thus, the whole procedure of LBM-DEM coupling is listed below:

1. Send DEM information, including particle position and particle velocity, to LBM.
2. Compute solid fraction, serving as ε_s in PSM, on lattice nodes according to particle position in LBM.
3. Solve LBM for fluid flow and compute $F_{hydrodynamic}$, $T_{hydrodynamic}$ and stresslet around the particles.
4. Solve DEM for particle motions with $F_{hydrodynamic}$ and $T_{hydrodynamic}$ calculated from LBM.
5. Repeat step 1.

Detailed simulation parameters will be presented in the following chapters.

Chapter 4

Rheology of suspensions composed of frictional and frictionless particles

In this chapter, simple shear flow of dense suspensions composed of frictional and frictionless particles is simulated using the discrete element method (DEM) for better understanding and tuning the viscosity of dense suspensions. We show that adding frictionless particles to suspensions of frictional particles decreases the relative viscosity of suspensions as a result of increased jamming volume fraction. However, the viscosity reduction is not as significant as that shown in experiments of suspensions containing rough and smooth particles, which means that the sliding friction alone is insufficient to describe the effect of particle roughness. Furthermore, when contacts between frictional and frictionless particles are treated as purely frictional or frictionless, the relationships between jamming volume fraction and fraction of frictional contact, f , are different. This indicates a scalar variable f , based on mean-field assumption of contacts, is inadequate in predicting the rheology of such binary systems and microstructure like contact network and force distribution should perhaps be taken into account.

4.1 Introduction

Dense suspensions consisting of solid particles immersed in a liquid are ubiquitous in industry. Understanding their rheology plays an important role in improving industrial processes. Among various industrial processes involving dense suspen-

sions, one of the common topics is understanding and tuning their viscosities by changing the surface properties of the particles or composition of suspensions.

As introduced in Section 2.2.2, the relative viscosity of suspensions η_r can be described by a solid volume fraction, ϕ , dependent function, and one of the most popular functions for suspensions with high solid volume fractions was proposed by Krieger and Dougherty [62]:

$$\eta = \eta_0 \left(1 - \frac{\phi}{\phi_J} \right)^{-\alpha} \quad (4.1)$$

where ϕ_J is the critical volume fraction, named jamming volume fraction in this chapter, where the viscosity diverges. The ϕ_J value depends on the friction coefficient, μ_p , between the particles: $\phi_J^{\mu_p \neq 0} \approx 0.60$ for $\mu_p = 0.5$ and $\phi_J^{\mu_p = 0} \approx 0.64$ for $\mu_p = 0$. The relationship between friction coefficients and jamming volume fractions can be found in Rangarajan et al. [109]. While this model works well for most suspensions, it does not include the possibility that suspensions exhibit non-Newtonian behavior such as shear-thickening, in which the viscosity increases η_r with shear stress σ or shear rate $\dot{\gamma}$. Various models have been proposed [133][12][15] to explain and predict shear thickening of suspensions, and a consensus that shear thickening results from the formation of frictional contacts has been achieved based on recent experiments and simulations[86][39][40]. Wyart and Cates [135] proposed a phenomenological model¹ that assumes the jamming volume fraction ϕ_J as a linear function of the fraction of frictional contacts, f :

$$\phi_J(f) = f \cdot \phi_m + (1 - f) \cdot \phi_{RCP} \quad (4.2)$$

where ϕ_m is $\phi_J^{\mu_p \neq 0}$ for frictional suspensions and ϕ_{RCP} is $\phi_J^{\mu_p = 0}$ for frictionless suspensions. The fraction of frictional contacts, f , can be estimated by a sigmoidal form in the shear thickening transition:

$$f(\sigma) = e^{-(\sigma^*/\sigma)^\beta} \quad (4.3)$$

Therefore, the full flow curve $\eta(\sigma)$ of shear thickening from simulation and experimental results [86][39] can be reproduced by combining Krieger-Dougherty relationship and Wyart-Cates(WC) model, i.e. Equation(4.1)(4.2)(4.3).

In this work, we introduce a binary model system composed of frictional and frictionless particles to elucidate the influence of surfactant coating, which is

¹Details about Wyart-Cates model can be found in Section 2.2.3

used to reduce the friction between particles, and test the applicability of the interpolated relationship between ϕ_J and f proposed by Wyart and Cates [135].

4.2 Numerical models

In this work, the discrete element method (DEM) with lubrication model, as introduced in Section 3.1.3, is employed to simulate the shear flow of a dense suspension of non-Brownian particles in a Newtonian solvent. The motion of each particle is captured by solving the Newton's motion equation:

$$m_i \frac{d\mathbf{x}_i^2}{dt^2} = \mathbf{F}_i^C + \mathbf{F}_i^H \quad (4.4)$$

The particle-particle contact interaction F^C is described by the linear Hooke spring model $F_n^C = k_n h$, with spring constant k_n and the extent of particle overlap h . The tangential spring force is $F_t^C = k_t h_t$, where $k_t = (2/7)k_n$, and the incremental tangential stretch h_t is initialized to 0 at contact and updated following Silbert et al. [119]. The relationship between normal component and tangential component of particle-particle contact force is restricted by the Coulomb criterion, $|F_t^C| \leq \mu |F_n^C|$, where μ is the friction coefficient between particles.

The hydrodynamic F^H interaction between fluid and particles includes the Stokes drag and short-ranged lubrication forces F^L between particles for dense suspensions. A simplified formulation of lubrication force for smooth particles and low Reynolds number flow is proposed by Radhakrishnan [108] and widely used in recent works[96][109].

Homogeneous simple shear flow at a constant shear rate $\dot{\gamma}$ was imposed by affine deformation in a three dimensional periodic domain with Lees-Edwards periodic boundary condition applied. The Stokes number $\rho_p \dot{\gamma} d^2 / \eta_f$ is kept much smaller than 1, where particle density ρ_p is the same as fluid density ρ_f , to ensure the inertial effect of particles is negligible. Additionally, the repulsive forces between particles are not included in our simulation, which indicates the rheology of this binary system is rate-independent.

The total stress was calculated by summing contributions from the contact, lubrication forces between particles and isolated particle stresslets:

$$\begin{aligned}
\boldsymbol{\sigma}^C &= \frac{1}{V} \sum_i \sum_{j>i} \mathbf{r}_{ij} \mathbf{F}_{ij}^C \\
\boldsymbol{\sigma}^L &= \frac{1}{V} \sum_i \sum_{j>i} \mathbf{r}_{ij} \mathbf{F}_{ij}^L
\end{aligned} \tag{4.5}$$

where V is the volume of the simulation box. The relative viscosity of the suspension is calculated from $\eta_r = \sigma / (\dot{\gamma} \eta_f)$, where σ is the xy component of the stress tensor in simple shear flow. All the results presented were obtained by averaging over at least 10 strain units in steady state.

Critical load model For capturing the shear-thickening behavior of suspensions by DEM, Mari et al. [86] proposed the critical load model (CLM). In this model, a threshold normal force F^{CL} is introduced to the friction law to capture the transition from frictionless to frictional contacts. When the normal contact force is smaller than this threshold force, particles interact as frictionless hard spheres. When the load is beyond the threshold, the contact is activated to be frictional. Thus, the friction law in CLM reads:

$$\left| \mathbf{F}_{C,\text{tan}}^{(i,j)} \right| \leq \begin{cases} \mu \left(\left| \mathbf{F}_{C,\text{nor}}^{(i,j)} \right| - F^{CL} \right) & \text{for } \left| \mathbf{F}_{C,\text{nor}}^{(i,j)} \right| \geq F^{CL} \\ 0 & \text{otherwise} \end{cases} \tag{4.6}$$

The CLM model is widely used to simulate shear thickening [95][86] and successfully reproduces the shear thickening curve for both CST and DST².

Friction between particles In our simulations of a binary model system, the friction coefficient μ is set to be 0.5 between frictional particles and 0 between frictionless particles. For the intermediate inter-species friction coefficient μ_{in} between frictional and frictionless particles, we consider two extreme conditions: $\mu_{in} = 0$ or $\mu_{in} = 0.5$ to make sure all frictional contacts are equivalent. In this way, there are only two different types of contacts in our simulation systems, frictionless contacts and frictional contacts with $\mu = 0.5$. It is easy straightforward to calculate the fraction of frictional contacts, which is denoted as f , by counting the number of frictional contacts and frictionless contacts.

²The critical load model is not implemented in the binary system we discussed in this chapter.

Sample preparation To avoid crystallization, $1800 \times (1 + \beta)$ bi-disperse frictional at diameter ratio 1:1.4 are generated in LAMMPS with nearly equal volumes, i.e. number ratio is 11:4. Here β is a proportional constant ($0 < \beta < 1$) that makes sure particle numbers for different sizes are integer for simplicity. The number ratio of frictionless particles is defined as:

$$\zeta = N_{\text{frictionless}} / (N_{\text{frictional}} + N_{\text{frictionless}}) = N_{\text{frictionless}} / N_p \quad (4.7)$$

where $N_{\text{frictionless}}$ is number of frictionless particles, $N_{\text{frictional}}$ is number of frictional particles, N_p is the total number of particles. By setting 1800 particles to be frictional and $1800 \times \beta$ to be frictionless, the number ratio $\zeta = \beta / (1 + \beta)$ ranges from 0 to 0.5. In contrast, the number ratio $\zeta = 1 / (1 + \beta)$ ranges from 0 to 0.5 by setting 1800 particles to be frictionless. In this way, we make sure the bi-dispersity holds and system size is limit in 1800-3600 particles for different ζ .

4.3 Results

4.3.1 Effect of adding frictionless particles

With the increase of the number fraction ζ of frictionless particles, where μ_{in} between frictional and frictionless particles is 0, the relative viscosity η_r decreases at fixed ϕ , as shown in Figure 4.1. The divergence of viscosity of this binary suspension at a fixed number fraction of frictionless particles ζ can be fitted by

$$\eta_r = A(\phi_J - \phi)^{-p} \quad (4.8)$$

where we fix $p = 2$, following previous simulation results[86][120][109] and leave A and ϕ_J as fitting parameters. Here ϕ_J , obtained by the Matlab tool: Curving Fitting, is the jamming volume fraction for the corresponding ζ of our binary system. To obtain more accurate fitting results, as the fluctuation of the suspension viscosity becomes large and the fitting equation, Equation 4.8, is quite sensitive close to the jamming point, we have done more simulations with volume fractions ϕ close to the fitting results ϕ_J^0 obtained from a regular sequence of volume fractions: 0.51, 0.53, 0.55, 0.57, 0.59, 0.61, 0.63. Figure 4.2 shows the simulation results and related fitting ϕ_J , denoted by dashed vertical lines. As

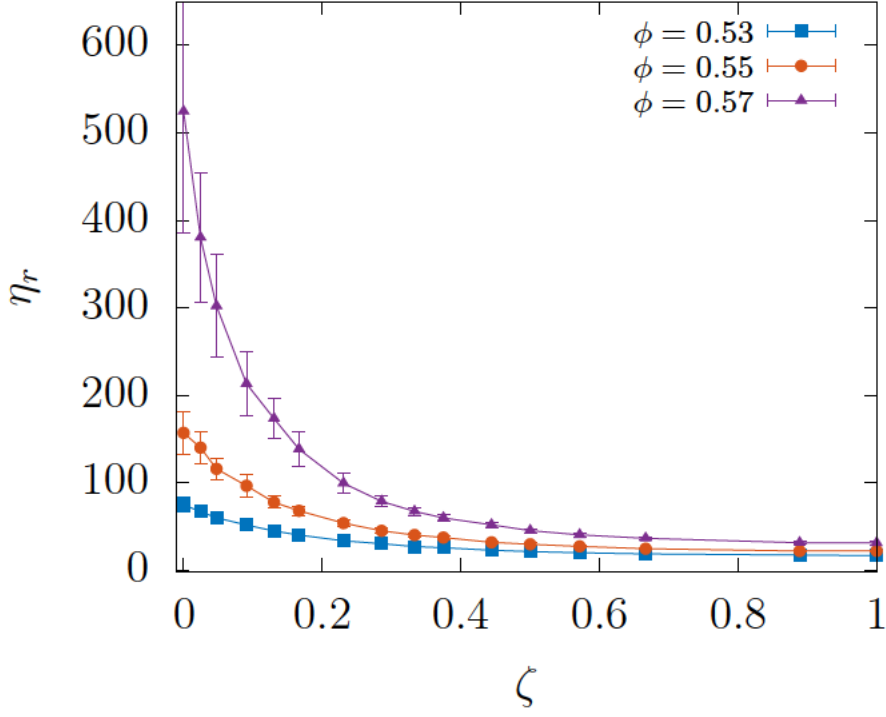


Figure 4.1 Relative viscosity η_r of suspensions (linear scale) at different number fractions ζ of frictionless particles with $\mu_{in} = 0$ for various volume fractions ϕ .

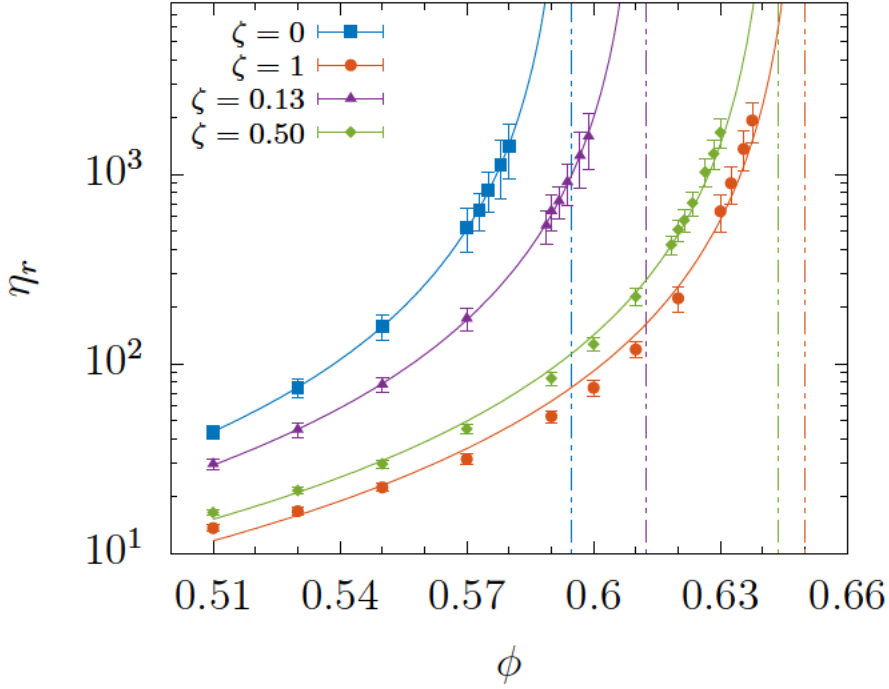


Figure 4.2 Relative viscosity η_r of suspensions as a function of different volume fractions for various values of ζ with inter-species friction coefficient $\mu_{in} = 0$. The jamming volume fractions ϕ_J for different values of ζ , indicated by the dot-dashed vertical lines, are obtained by fitting η_r with Equation 4.8. Symbols are simulation results.

ζ varies from 0 to 1, ϕ_J moves from 0.595 for a purely frictional system with $\mu = 0.5$, to 0.65 for a purely frictionless system, agreeing with previous work [109].

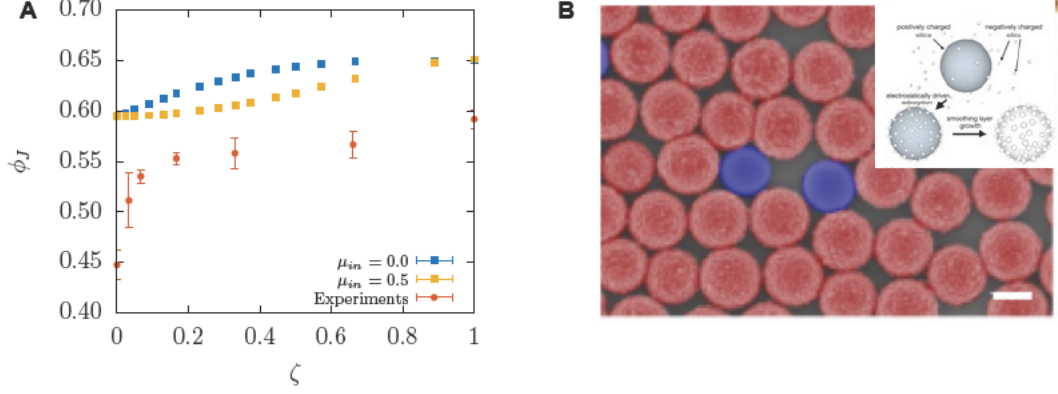


Figure 4.3 (A) Comparison between simulation and experimental results. Jamming volume fractions ϕ_J of simulation results for $\mu_{in} = 0.0$ (blue solid square), $\mu_{in} = 0.5$ (yellow solid square) and experimental results[48] (red solid circle) as a function of number fractions ζ . (B) SEM image of a suspension containing 33% of smooth particles taken from Hsu et al. [48]

From simulation results of our model system, we found that reducing some particles' friction can decrease the relative viscosity η_r and the jamming volume fraction ϕ_J of the suspension, as shown in Fig 4.2. The relationship between ζ and ϕ_J for $\mu_{in} = 0.0$ and $\mu_{in} = 0.5$ are shown in Fig 4.3. We can observe that ϕ_J for purely frictional, $\zeta = 0$, or frictionless, $\zeta = 1$ systems are the same but the increase trends are quite different for different μ_{in} . The main effect of ϕ_J is seen within 0% $\sim$ 30% for $\mu_{in} = 0$ whereas the range changes to 30% $\sim$ 60% for $\mu_{in} = 0.5$.

To better understand the role of sliding friction in our binary system, we compared our results qualitatively with the experimental results about the mixture of smooth and rough particles by Hsu et al. [48]. Here we are not aim to reproduce precisely the experimental conditions, where the friction of particles came from the roughness of surface, as shown in Fig 4.3B. They showed the change of ϕ_J with different mixture ratios of smooth particles, noted by solid red circles in Fig 4.3A. However, jamming volume fraction for experimental mixtures of smooth and rough particles exhibits more remarkable variance than our model system, where 3% of smooth particles can increase ϕ_J by 6%. Moreover, ϕ_J for $\zeta = 0$

in experiments is around 0.44, which is much lower than our system, $\phi_J = 0.595$ for $\mu = 0.5$ and even lower than previous work [109][118][126], where ϕ_J lies within 0.54 and 0.57 for $\mu = 10$, which indicates that such friction coefficient defined by the Coulomb criterion, $|F_t^C| \leq \mu|F_n^C|$, which represents the constraint of sliding between particles, used in our simulations is not sufficient to describe the effect of particles roughness produced by Hsu et al. [48]. Such raspberry-like surface roughness can constrain the freedom of sliding, rolling and twisting and hence influence the contact network and space distribution of the mixture of rough and smooth particles, which can not be observed in our simulation. Recently, Blair and Ness [7] reproduced similar viscosity curves as Hsu et al. [48] by simulating aggregate particles, which captures the physical interlocking of particles and suggests that roughness introduces other constraints such as rolling and twisting.

4.3.2 Comparison with Wyart-Cates model

In our binary model system, f can be calculated directly by judging types of particles getting into contact. We also calculated f by counting contacts with or without tangential force, which produced exactly the same results as the previous method. The relationships between f and ζ for different μ_{in} is shown in Fig 4.4 and can be fitted perfectly by:

$$f \approx \begin{cases} (1 - \zeta)^2 & \mu_{in} = 0 \\ 1 - \zeta^2, & \mu_{in} = 0.5 \end{cases} \quad (4.9)$$

The form of Equation 4.9, which was also found in Trulsson et al. [129], demonstrates that probabilities for two *random* particles getting into contact are the same and particles are identical in the simulation, which means such mixture of frictional and frictionless particles can not induce phase separation even after a large shear strains ($\gamma > 20$). Figure 4.4B shows that f is independent of the volume fraction ϕ .

Based on the discussion above, we can get the relationship between f , counted from simulation directly as shown in Figure 4.4 A, and corresponding ϕ_J , fitting results from Figure 4.2 and Equation 4.8. As shown in Figure 4.5, the linear interpolation of the WC model, $\alpha = 1$ for the purple line, does not produce a

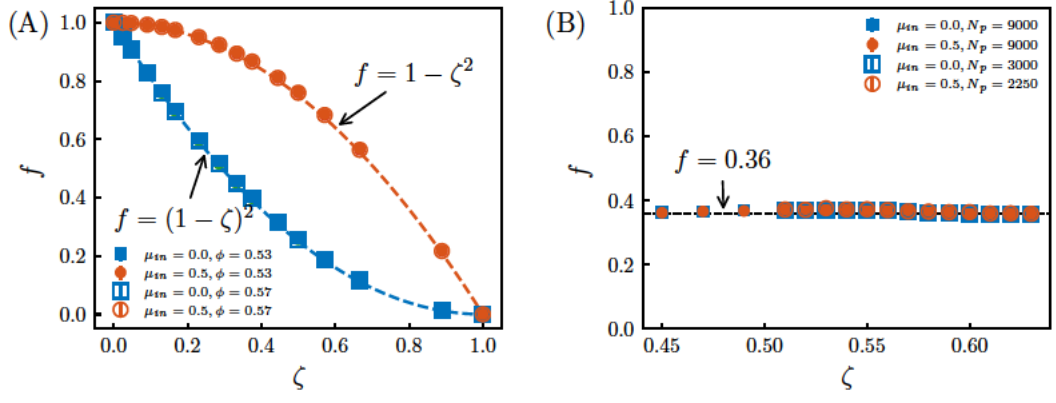


Figure 4.4 (A) Fraction of frictional contacts f as a function of number fraction ζ for different volume fractions, $\phi = 0.53$ (blue squares) and $\phi = 0.57$ (red circles), and different intermediate friction coefficient between frictional and frictionless particles, $\mu_{in} = 0.0$ (solid points) and $\mu_{in} = 0.5$ (empty points). The red and blue dashed lines are obtained from Equation 4.9. (B) Symbols are simulation results, and dashed lines are $f=0.36$ calculated from Equation 4.9.

good fit for our results. Whereas a modified non-linear interpolation:

$$\phi_J = \phi_m f^\alpha + \phi_{RCP}(1 - f^\alpha) \quad (4.10)$$

produces a better fit. The values of the fitting parameter α are different for different cases: $\alpha = 1$ for shear thickening indicted by WC model, $\alpha = 1.5$ for $\mu_{in} = 0$ and $\alpha = 2$ for $\mu_{in} = 0.5$, which means ϕ_J for the same f are different for these three cases. At a given f , $\phi_J^{ST} < \phi_J^{\mu_{in}=0} < \phi_J^{\mu_{in}=0.5}$, and $\eta_r^{ST} > \eta_r^{\mu_{in}=0} > \eta_r^{\mu_{in}=0.5}$ for the same ϕ .

As shown in Figure 4.6, η_r from simulations of shear thickening by CLM³ is higher than the other two and η_r for $\mu_{in} = 0.0$ is also higher than $\mu_{in} = 0.5$, which is more obvious in higher ϕ close to jamming. Here each empty square point represents f and η_r calculated from one timestep of a series of CLM simulations with the same ϕ and different shear rates $\dot{\gamma}$ as the fluctuations are relatively large for f and η_r in shear thickening suspensions.

³Here the simulations using CLM is for comparing with our binary system and the friction coefficient μ in Equation(4.6) is set to be 0.5.

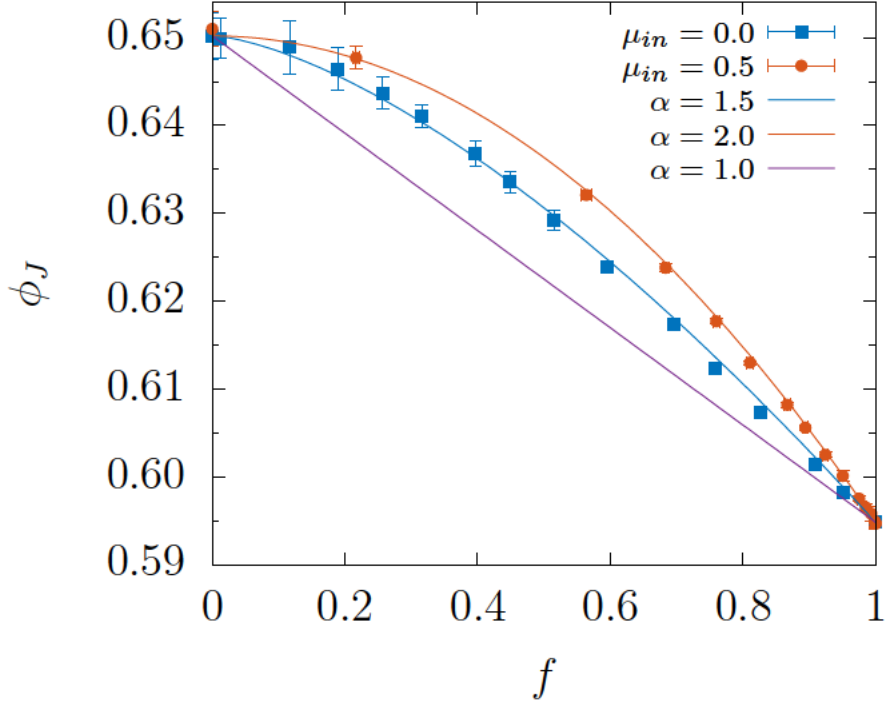


Figure 4.5 Relationship between f and ϕ_J for $\mu_{in} = 0.0$ (blue solid square with error bar) and $\mu_{in} = 0.5$ (red solid square with error bar), solid lines are generated from Equation 4.10 with different fitting parameter α

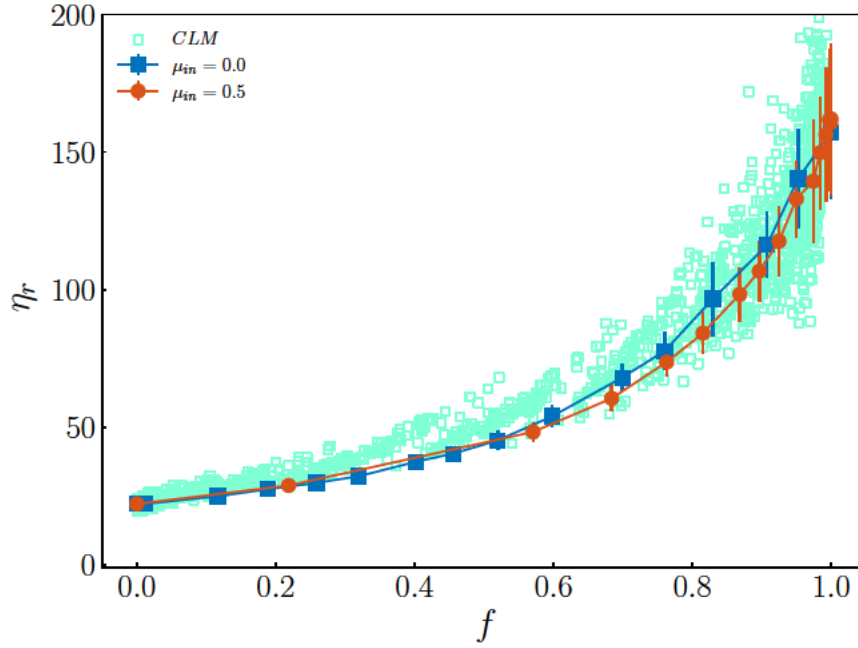


Figure 4.6 η_r as a function of f for different cases: $\mu_{in} = 0$ (blue solid square with error bar), $\mu_{in} = 0.5$ (red solid square with error bar) and CLM for shear thickening (aquamarine empty square) when $\phi = 0.55$.

4.3.3 Microstructure for different cases

The difference between shear thickening suspensions and binary suspensions in our work is obvious in microstructure, especially the distribution of frictional contacts. Figure 4.7A is a snapshot of the 2D simulation of the CLM model. Frictional contacts, in which normal forces are larger than F^* , the threshold force value in CLM, are coloured by black nodes. For the binary system with $\mu_{in} = 0$, we randomly choose some particles to be frictional and get the sketch figure as Figure 4.7B. Frictional particles are represented by red circles, and the contacts with strong normal force ($F_n > F^*$) can either be frictional or frictionless depending on the types of particles coming into contact. The frictional contacts in shear thickening are determined by the strength of the normal force and evolve with the force chain, whereas frictional contacts in our binary system are strictly constrained by the distribution of frictional particles.

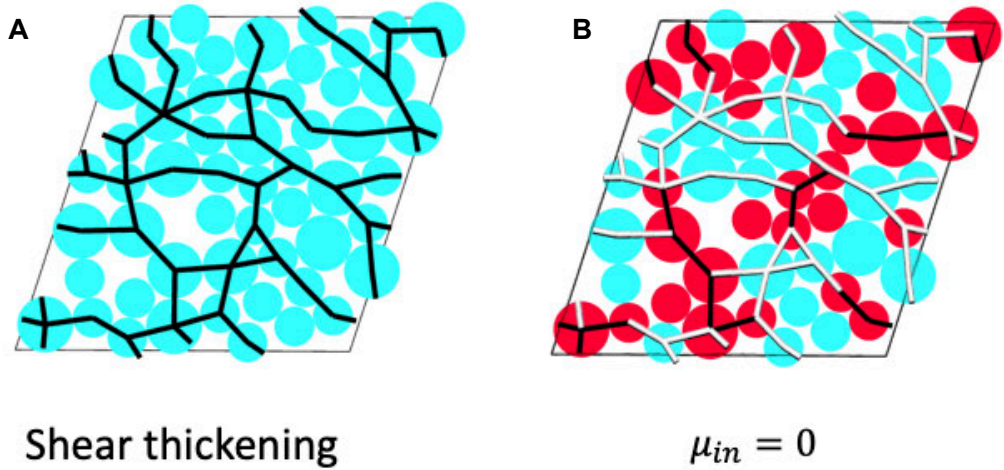


Figure 4.7 Sketches of 2D force chains in (A). shear thickened suspensions, (B). binary system with $\mu_{in} = 0$. Black lines represent frictional contacts, and white lines represent frictionless contacts. Blue circles in B represent frictionless particles, and red circles in B represent frictional particles.

For exploring the difference between binary systems with different μ_{in} , larger systems containing 9000 particles with $\zeta = 0.4$ for $\mu_{in} = 0$ or $\zeta = 0.8$ for $\mu_{in} = 0.5$, ensuring $f \approx 0.36$ for different cases, are simulated under different volume fractions. The difference of ϕ_J , $\Delta\phi_J = \phi_J^{\mu_{in}=0.5} - \phi_J^{\mu_{in}=0}$, between these two cases is around 0.013 for $f \approx 0.36$ according to Equation 4.10, where $\phi_J^{\mu_{in}=0.5} \approx 0.643$ and $\phi_J^{\mu_{in}=0} \approx 0.63$. The difference between these two cases is minor until the high

volume fraction close to ϕ_J . Figure 4.8A is the probability distribution for the non-affine velocity of frictional particles, which exhibits a difference in the tail part, $\delta V / \langle \delta V \rangle > 3$, of PDF for $\phi = 0.62$ whereas the difference of PDF for all the particles is small, as shown in the inset figure. The mobility of contacts, which means the particle overcomes the sliding constraint and is defined as $F_t > \mu F_n$, also exhibits obvious differences for different μ_{in} . However, both the tail part of PDF of non-affine velocity and the mobility of contacts, shown in Figure 4.8, only take up less than 5% of the whole system, and the difference between these physical quantities cannot directly reveal the difference between different μ_{in} . The relationship between fitting parameters α and microstructure differences for these

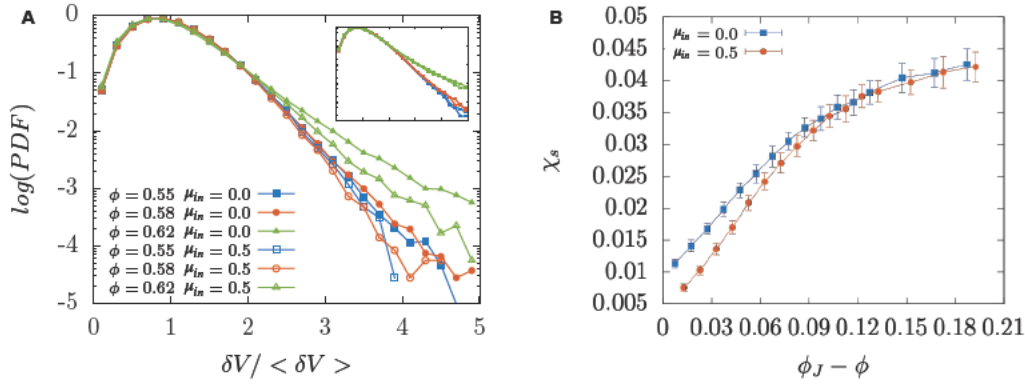


Figure 4.8 (A) Probability distribution of non-affine velocity of frictional particles for different μ_{in} . Inset: probability distribution for all the particles. (B) Relationship between mobility χ_s , defined as the fraction of sliding contacts within frictional contacts, and $\phi_J - \phi$.

According to the discussion above, we would expect particles within strong force chains to carry the largest loads and contribute the most to the stable packing. In shear thickening, we expect all the frictional contacts to be activated by the strong normal force and stabilize the force chains. However, in the binary system, the distribution of frictional contacts is determined by the distribution of frictional particles, which means part of the frictional contacts contributes less to the stabilization of the packing if they are not aligned with the strong force chains. Therefore, the contribution of frictional contacts has to be distinguished according to their space distribution. For the same f , case $\mu_{in} = 0$ has more frictional particles than case $\mu_{in} = 0.5$, which means the possibility for frictional contacts located in the strong force chain is higher for $\mu_{in} = 0$. Here we give a possible explanation of the non-linear interpolation of f , but we cannot figure

out whether the fitting parameter α has deeper physical meaning or it is entirely fortuitous.

We have to emphasize that the WC model is designed to reveal the consequences of a simplified set of assumptions in the most perspicuous way, and (according to its authors[135]) not meant for the fitting of data[41]. Our work here is just to explore the capability of the WC model for more general systems. A failure of the WC model to its inability to distinguish large-large, large-small and small-small frictional contacts in a strongly bi-disperse system with a large diameter ratio(1:4) was reported in Guy et al. [41], which also supports that more details about particle properties and microstructural details should be taken into consideration for applying WC model to predict jamming volume fraction and suspension rheology.

4.4 Conclusions

This work simulated a binary system composed of frictional and frictionless particles. The relative viscosity of such a system can be reduced by adding frictionless particles, which provides a possible method to tune the viscosity of dense suspension by adding some smooth (frictionless) particles. The viscosity of such a binary system also obeys the Krieger and Dougherty relationship, and the jamming volume fractions are determined by the ratio of frictionless particles ζ .

A non-linear interpolation of f based on the WC model is employed here to fit ϕ_J and f of the binary system. Furthermore, different friction coefficients between frictional and frictionless particles result in different fitting values α , which indicates a single parameter, f , which is of mean-field nature is not sufficient to predict the rheology of such binary suspensions composed of frictional and frictionless particles. Future work to bridge the bulk rheology and microstructure, such as force distribution and contact network, is warranted.

For further investigation of this binary system, 2D simulations are suggested for measuring the microstructure quantitatively, such as contact network and force chain, and checking the capability of fitting parameter α .

Chapter 5

Simulations of sheared suspensions by LB-DEM

In this chapter, we first summarise the simulation details of our coupled lattice Boltzmann discrete element method (LBDEM). Then the simple sheared suspensions are simulated by LBDEM and DEM, which includes short-range lubrication force and stokes drag force. The simulation results are compared, including viscosity, contact number and velocity profiles from these two approaches. The constitutive relationships proposed by Krieger and Dougherty [62] and Boyer et al. [11] are employed to fit our simulation results for obtaining the jamming volume fraction and critical macroscopic friction coefficient. The shear thickening behaviour is also captured by LBDEM simulations and compared with the results from DEM simulations.

5.1 Numerical model and simulation details

5.1.1 Discrete element method

The discrete element method, related to molecular dynamics, is a widely used particle-based simulation method in engineering processes. As introduced by Cundall and Strack [21], DEM is based on Newton's equations integrating in time for translational and rotational motion of particles, considering particle interactions, such as elastic force and friction. The equations describing the

translational and rotational motion read:

$$m_i \frac{d\mathbf{x}_i^2}{dt^2} = \mathbf{F}_i^C + \mathbf{F}_i^H + \mathbf{F}_i^L \quad (5.1)$$

$$J_i \frac{d\boldsymbol{\omega}_i}{dt} = \mathbf{T}_i^C + \mathbf{T}_i^H + \mathbf{T}_i^L \quad (5.2)$$

where m_i , $\mathbf{x}_i$, J_i and $\boldsymbol{\omega}_i$ are the mass, position, moment of inertia and angular velocity of an individual particle i , respectively. $\mathbf{F}$ and $\mathbf{T}$ are the force and the torque acting on each particle, including a mechanical contact ($\mathbf{F}^C$ and $\mathbf{T}^C$) when particles overlap, a lubrication interaction ($\mathbf{F}^L$ and $\mathbf{T}^L$) provided by the surrounding fluid when the surface separation between particles is sufficiently small compared to the particle size[36] and a hydrodynamic interaction ($\mathbf{F}^H$ and $\mathbf{T}^H$) resulting from the interaction between particles and fluid.

In this work, the mechanical contact between particles is modelled through a spring-dashpot model in normal as well as tangential contact direction. Details about the spring-dashpot model can be found in Section 3.1.2.

In our DEM simulations, the short-range lubrication force is described by a simplified formula of lubrication force, Equation(3.15), proposed and implemented into LAMMPS and LIGGGHTS by Radhakrishnan [108]. The hydrodynamic force is captured by a drag force from the relative fluid and particle motion, which is based on the Stokes drag law of a single sphere. Thus $\mathbf{F}^H$ and $\mathbf{T}^H$ can be written as:

$$\mathbf{F}_{\text{Stokes}} = 6\pi\eta_f r_p (\mathbf{u}_f^\infty(\mathbf{x}_p) - \mathbf{u}_p) \quad (5.3)$$

$$\mathbf{T}_{\text{Stokes}} = 8\pi\eta_f r_p (\boldsymbol{\omega}_f^\infty(\mathbf{x}_p) - \boldsymbol{\omega}_p) \quad (5.4)$$

The fluid rotation is $\boldsymbol{\omega}_f^\infty(\mathbf{x}_p) = \frac{1}{2} (\nabla \times \mathbf{u}_f^\infty(\mathbf{x}_p))$ and for a sheared system, a linear velocity profile for the fluid velocity can be assumed, i.e. the only non-zero components for the strain rate tensor are $\dot{\Gamma}_{xy} = \dot{\Gamma}_{yx} = \frac{1}{2}\dot{\gamma}$.

In a suspension, the drag force acting on a sphere is influenced by the presence of other particles, leading to a reduction in the effective viscosity of the fluid. To account for this effect, a hindrance function is typically introduced. A detailed description of hindrance functions can be found in Section 6.1.1. However, in our DEM approaches, we have already included pairwise lubrication interactions and contacts between particles, which influence the particle motion and are included

in the hindrance function implicitly. Therefore, the drag forces acting on the particles in our simulation are calculated using the conventional Stokes drag law of a single sphere, rather than a modified drag force based on the hindrance function.

Stress calculation of DEM

The total bulk stress is decomposed into different contributions: Mechanical particle-particle contact stress $\boldsymbol{\sigma}^C$ and contributions based on the lubrication force $\boldsymbol{\sigma}^L$. For inter-particle forces, such as contact forces or lubrication forces, the stress computation can be described as:

$$\boldsymbol{\sigma}^C = \frac{1}{V} \sum_i \sum_{j>i} \mathbf{r}_{ij} \mathbf{F}_{ij}^C \quad (5.5)$$

and

$$\boldsymbol{\sigma}^L = \frac{1}{V} \sum_i \sum_{j>i} \mathbf{r}_{ij} \mathbf{F}_{ij}^L \quad (5.6)$$

where $\mathbf{r}_{ij}$ is the vector pointing from particle j to i . The stress caused by the hydrodynamic force, which is assumed to be a single sphere Stokes drag force, should also be considered in the stress evaluation for which the stresslet could be expressed according to the single sphere stresslet [36]:

$$\mathbf{S} = -\frac{20}{3} \pi \eta_f r_p^3 \dot{\mathbf{\Gamma}}^\infty. \quad (5.7)$$

Under simple shear, the bulk shear and normal stresses (pressure), σ_{xy} and P , can be obtained by summing the contributions σ_{xy}^i and P^i , where $P^i = \frac{1}{3} (\sigma_{xx}^i + \sigma_{yy}^i + \sigma_{zz}^i)$

5.1.2 Lattice Boltzmann Method

The Lattice Boltzmann Method (LBM), a lattice-based model unlike DEM, is a class of computational fluid dynamics (CFD) methods for complex fluid simulations. Basically, the fluid can be described as the sum of the probability density function $f(\mathbf{x}, \mathbf{u}, t)$, which determines the probability density of finding a particle with velocity $\mathbf{u}$ at position $\mathbf{x}$ at time t . The evolution of the discretized

Boltzmann equation on each lattice can be interpreted as the propagation and collision part:

Propagation part:

$$f_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) = f_i(\mathbf{x}, t + \Delta t) \quad (5.8)$$

Here, the set of $\mathbf{c}_i$ is the lattice velocities which should be chosen carefully to retrieve the equations for mass and momentum. In this work, D3Q19 is chosen for the velocity set in the simulation.

Collision part:

$$f_i(\mathbf{x}, t + \Delta t) = f_i(\mathbf{x}, t) + \Omega_i^{BGK} \quad (5.9)$$

Here Ω_i^{BGK} is the simplest approximation of the collision between particle distribution functions. The approximation term, proposed by Bhatnagar et al. [6] and named as Bhatnagar-Gross-Krook (BGK) collision, assumes that the particle distribution function f is relaxed towards a local equilibrium f_{eq} over a collision relaxation time τ , i.e.

$$\Omega_i^{BGK} = \frac{\Delta t}{\tau} (f_i^{eq}(\mathbf{x}, t) - f_i(\mathbf{x}, t)) \quad (5.10)$$

where τ is the dimensionless relaxation parameter and the equilibrium distribution function $f_i^{eq}(\mathbf{x}, t)$ is:

$$f_i^{eq}(\mathbf{x}, t) = w_i \rho \left(1 + \frac{\mathbf{u} \cdot \mathbf{c}_i}{c_s^2} + \frac{(\mathbf{u} \cdot \mathbf{c}_i)^2}{2c_s^4} - \frac{\mathbf{u} \cdot \mathbf{u}}{2c_s^2} \right) \quad (5.11)$$

where ω_i is the weight specific to the chosen velocity set. ρ and $\mathbf{u}$ are, respectively, the macroscopic fluid density and velocity and can be calculated from: $\rho = \sum_i f_i$ and $\rho \mathbf{u} = \sum_i f_i \mathbf{c}_i$. $c_s = c/\sqrt{3}$ is the lattice sound speed where $c = \Delta x/\Delta t$ is the lattice speed. The fluid pressure field p is determined by the relationship: $p = c_s^2 \rho$. The fluid kinematic ν is determined by the discretisation and numerical parameters for recovering the Navier-Stokes equation:

$$\nu = \frac{1}{3} \left(\tau - \frac{1}{2} \right) \frac{(\Delta x)^2}{\Delta t} \quad (5.12)$$

Here Δx is the basic unit for lattice spacing, and Δt is the basic unit of the time step, which represent a spatial resolution and a time resolution, respectively. From Equation (5.12), we can find that the simulation time step is determined

by the fluid viscosity and lattice size in LBM.

5.1.3 Fluid-solid coupling

Various methods have been proposed to handle the hydrodynamic interaction between fluid and suspended solid particles. This work uses the partially saturated cell method (PSM) proposed by Noble and Torczynski [99].

In PSM, an additional collision term Ω^s is introduced to include interactions between a solid particle and particle distribution functions on a lattice node. The fluid and solid phases are differentiated by a weighting function for the solid phase, which leads to the modified LBM equation:

$$f_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) = f_i(\mathbf{x}, t) + [1 - B(\mathbf{x}, \tau)]\Omega_i^f + B(\mathbf{x}, \tau)\Omega_i^s \quad (5.13)$$

where $\Omega_i^f = \frac{\Delta t}{\tau} f_i(\mathbf{x}, t) - f_i^{eq}(\mathbf{x}, t)$ for BGK collision operator and $B(\mathbf{x}, \tau)$ is a weighting function related to the solid fraction ϵ_s of the lattice node at $\mathbf{x}$. The solid fraction ϵ_s is calculated from the sub-cell method, which is presented in Section 3.3.3. Here we choose a linear expression for the weighting function $B(\mathbf{x}, \tau)$, which reads:

$$B(\mathbf{x}, \tau) = \epsilon_s \quad (5.14)$$

The solid collision term, named as super-position method, reads:

$$\Omega_i^s = f_i^{eq}(\mathbf{u}_s) - f_i + (1 - \frac{\Delta t}{\tau})(f_i - f_i^{eq}(\mathbf{u})). \quad (5.15)$$

A detailed analysis of the accuracy of the super-position method in calculating the stresslet and suspension viscosity refers to Najuch and Sun [93].

The hydrodynamic force and torque ($\mathbf{F}^H$ and $\mathbf{T}^H$) on a particle can be obtained by summation of the solid phase collision term multiplied by the lattice velocities over all lattice nodes covered by a particle:

$$\mathbf{F}^H = \frac{h^d}{\Delta t} \sum_n B_n \sum_i \Omega_i^s \mathbf{c}_i \quad (5.16)$$

and

$$\mathbf{T}^H = \frac{h^d}{\Delta t} \sum_n (\mathbf{x} - \mathbf{x}_s) \times \left(B_n \sum_i \Omega_i^s \mathbf{c}_i \right) = \sum_n (\mathbf{x} - \mathbf{x}_s) \times \mathbf{F}^H, \quad (5.17)$$

where h is the lattice spacing in d dimensions.

Lubrication correction

The LBM has a limited spatial resolution, i.e. the lattice size Δx , which means that lubrication forces between particles can be only resolved to particle-particle gap distances of around one lattice cell width. For smaller gap distances, a lubrication force correction is necessary to model the hydrodynamic particle-particle interactions. Therefore, the lubrication force correction is employed in this work, and the related expression reads:

$$\mathbf{F}_{\alpha, \text{correction}}(\beta, \xi) = \mathbf{F}_{\alpha}(\beta, \xi) - \mathbf{F}_{\alpha}(\beta, \delta_{\text{cut}} \xi_N), \text{ for } \xi \leq \delta_{\text{cut}} \xi_N = \delta_{\text{cut}} h_{\text{lattice}} \quad (5.18)$$

where $\beta = d_i/d_j$ is the particle size ratio, $\xi = \Delta x/d_p$ is the dimensionless gap distance and δ_{cut} is a cut-off calibration parameter for the lubrication force correction. Following the analysis by Najuch [94], we choose the cut-off parameter δ_{cut} as 0.75, 0.05 and 0.1 for normal, tangential and rotational components, respectively, when collision relaxation parameter τ is set to be 0.65.

In LBDEM simulations, the lubrication force models are based on the grand-resistance matrix, which is introduced in Section 3.1.3, and explicit formulations of the components in the matrix can be found in Kim and Karrila [58] and appendix in Mari et al. [86].

Stresslet calculation

In our LBDEM simulations, the stress contributions from contact force and lubrication force are the same as DEM, except the lubrication force in LBDEM is corrected, i.e. $\mathbf{F}_{\text{correction}}^L$. The stresslet in LBM can be computed from the hydrodynamic lattice forces, Equation (5.16), by summing over all particle-covered lattice nodes and particles:

$$\begin{aligned} \sigma_{\alpha\beta, \text{stresslet}} &= -\frac{1}{V} \sum \int_{A_p} \frac{1}{2} (\sigma_{\alpha\gamma} x_{\beta} + \sigma_{\beta\gamma} x_{\alpha}) n_{\gamma} dA \\ &= -\frac{1}{V} \sum^{N_{\text{particles}}} \sum^{N_{\text{nodes}}} \left(\frac{1}{2} (F_{\alpha\gamma}^{LBM} x_{\beta} + F_{\beta\gamma}^{LBM} x_{\alpha}) \right) \end{aligned} \quad (5.19)$$

where the vector $\mathbf{x}$ points from the particle centre to the lattice node on which F^H , calculated from LBM, acts. The negative sign ensures the stresslet computation is consistent to the stresses stemming from particle-particle interactions.

5.1.4 Simulation setup

For the simulation of suspensions under simple shear flow, Lees-Edwards boundary conditions for DEM and LBDEM, introduced in Section 3.2.4, were imposed on a three-dimensional periodic domain. The particle distribution was bi-disperse with diameters to be $1.4 d_p$ and d_p and a volume ratio to be 1:1. The simulation domain size was chosen to be $[12d \times 12d \times 12d]$ to minimise boundary effects. Thus, the numbers of particles with different diameters are determined by the volume fraction ϕ and volume ratio. The simulation box is deformed with a constant shear rate $\dot{\gamma}$, which ensures the Reynolds number of the suspension $Re = \rho_f \dot{\gamma} d_p^2 / \eta_f = 0.1$.

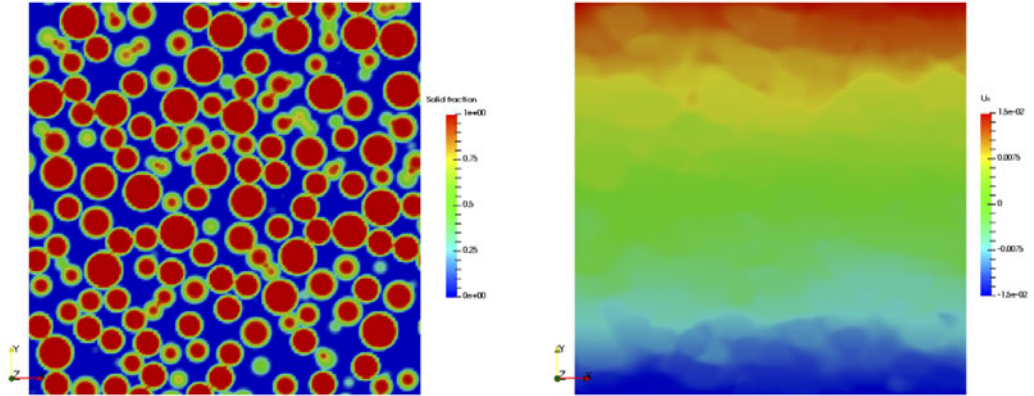


Figure 5.1 Snapshots of a LBDEM simulation of a simple sheared suspension with $\phi = 0.5$ and $Re = 0.1$. The left figure shows the distribution of solid fractions, and the right figure shows the fluid velocity in the sheared direction.

5.2 Results

5.2.1 Viscosity of sheared suspensions

In this work, simulations of sheared suspensions with a different friction coefficient of solid particles, $\mu_p = 0$ and $\mu_p = 0.5$, were performed with the above-described LB-DEM coupling. Results are compared to DEM simulations, for which only short-range lubrication and Stokes drag were taken into consideration.

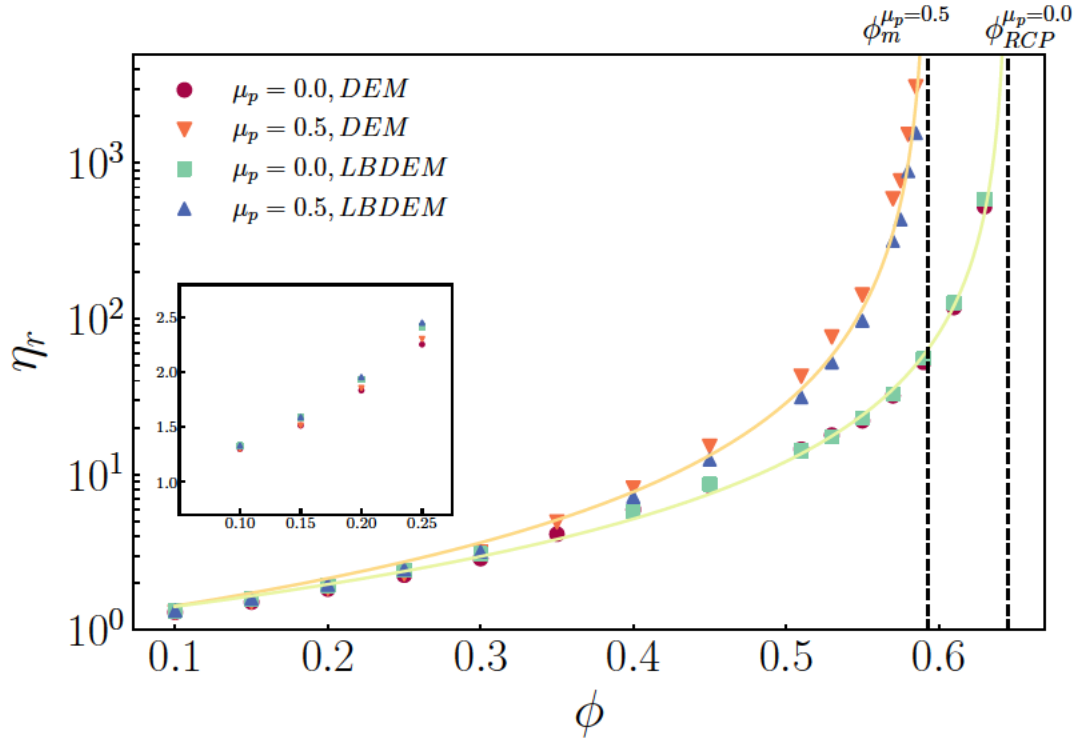


Figure 5.2 Relative viscosity values η_r for different volume fractions ϕ obtained from LBDEM and DEM simulations of simple sheared suspensions. Inset is viscosity values for low volume fractions. Vertical dashed lines indicate the critical volume fractions $\phi_{RCP} = 0.645$ and $\phi_m = 0.593$ for $\mu_p = 0$ and $\mu_p = 0.5$, respectively.

As shown in Figure 5.2, the suspension viscosity increases with the solid volume fraction. Similar to existing simulation results[86], there are clearly two $\eta_r(\phi)$ curves which diverge at two different critical volume fractions for frictional ($\mu_p = 0.5$) and frictionless ($\mu_p = 0$) particles. The critical volume fractions can be obtained by fitting our results against the well-known Krieger-Dougherty

relationship[62]:

$$\eta_r = A(\phi_m - \phi)^{-\alpha} \quad (5.20)$$

Here the fitting results for LBDEM simulations are $\phi_m = 0.593, \alpha = 1.8$ for frictional particles, $\mu_p = 0.5$, indicated by the yellow line in Figure 5.2, and $\phi_{RCP} = 0.645, \alpha = 1.62$ for frictionless particles, indicated by the green line. The fitting results α are slightly different from the usually used parameter $\alpha = 2$, as mentioned in Section 2.2, but the critical volume fractions, i.e. jamming volume fractions, are in good accordance with available results [86],[37][109],[31].

The inset figure of Figure 5.2 shows the differences of suspension viscosities calculated from DEM and LBDEM simulations for intermediate volume fractions ($0.15 < \phi < 0.25$). The viscosity difference mainly comes from the long-range hydrodynamic interactions, which are not included in our DEM simulations. Moreover, the viscosity values in this region, especially when $\phi < 0.2$, are close for frictional and frictionless suspensions, which indicate that frictional contacts in this region, in which averaged contact number is no more than 0.5 from Figure 5.3, is not essential to the rheology of the suspensions, compared to hydrodynamic interactions. The For higher volume fractions, the stress contribution from particle contacts overruns the long-range hydrodynamic interactions in such a way that the viscosities of frictionless suspensions with $\phi > 0.4$ are the same for LBDEM and DEM simulations.

However, the viscosity results from DEM simulations for frictional suspensions, $\mu_p = 0.5$, are higher than those from LBDEM in the high volume fraction region ($\phi > 0.4$). Najuch [94] reported a similar difference for $\mu_p = 1$ and compared the stress contributions, including contact, lubrication and stresslet in detail. The contact stress is larger for DEM than for LBDEM simulations, which is also reported by Gallier et al. [31], in which a comparison between fully resolved Stokes equations (FS) and Molecular Dynamics (MD) with short-range lubrications was conducted, and MD overestimated contact stresses than FS. However, the comparison of averaged particle contact number, which is directly related to the contact stresses, was not found in both of them. Here the results of contact number Z are presented in Figure 5.3. We can find that Z is larger in DEM simulations than in LBDEM simulations, either for frictional or frictionless particles. Unfortunately, a reason for differences in the contact stress contributions has not been found and would require further investigations.

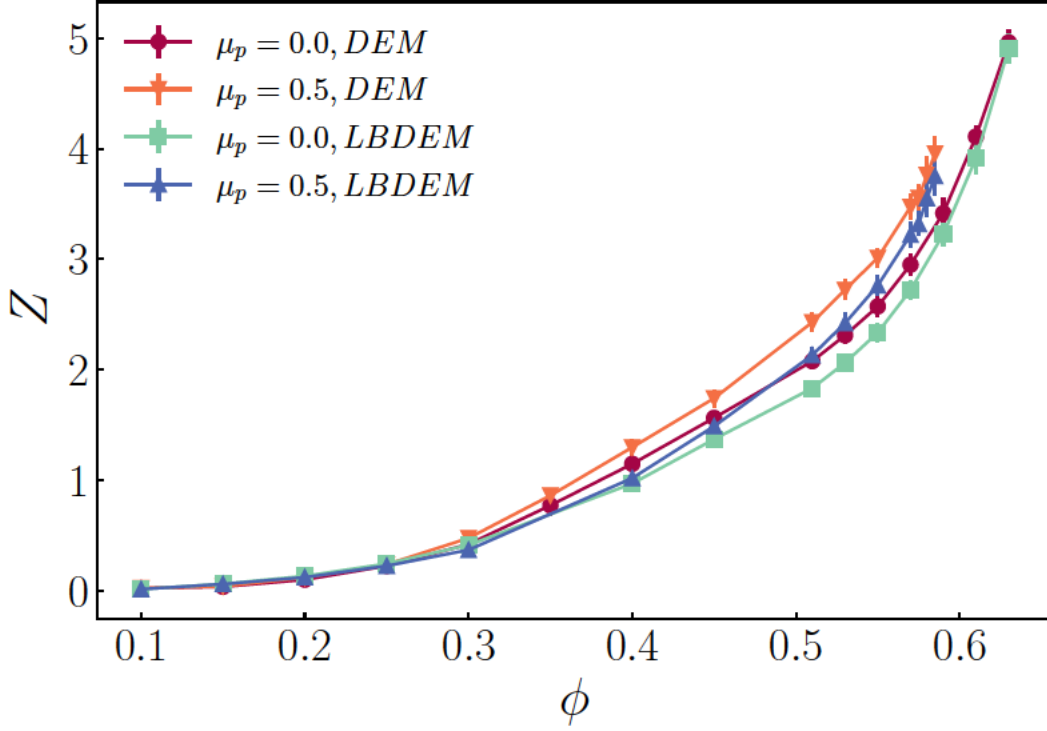


Figure 5.3 Averaged contact numbers Z of particles for different ϕ .

Contact number As reported by Rangarajan et al. [109] and Silbert [118], the contact number increases to a critical value Z_J as $\phi \rightarrow \phi_J^\mu$. Z_J is expected to be 6 for frictionless particles and 4 for frictional particles with $\mu \rightarrow \infty$, according to the Edwards statistical ensemble packing theory[40]. Here we have shown contact numbers in our simulations for ϕ close to ϕ_J^μ in Table 5.1 and 5.2. Here we estimate our Z_J according to a linear extrapolation of data listed in the tables. With fitted critical volume fractions $\phi_m = 0.593$ for $\mu_p = 0.5$ and $\phi_{RCP} = 0.645$ for $\mu_p = 0$, the estimated critical contact numbers are $Z_J^{\mu_p=0.5} \approx 4.2$ and $Z_J^{\mu_p=0} \approx 6.4$. The estimated values are similar to Z_J reported in a weak bi-disperse suspension system with a particle size ratio of 1.4:1[109].

ϕ	0.57	0.575	0.58	0.585
DEM	3.47	3.55	3.76	3.96
LBDEM	3.22	3.32	3.55	3.75

Table 5.1 Contact numbers for $\mu_p = 0.5$

Velocity profiles In Figures 5.4, the time and space averaged velocity profiles with respective solid fractions of $\phi = 0.15$, $\phi = 0.3$, $\phi = 0.5$, $\phi = 0.57$ are

ϕ	0.57	0.59	0.61	0.63
DEM	2.95	3.42	4.11	4.96
LBDEM	2.72	3.22	3.92	4.91

Table 5.2 Contact numbers for $\mu_p = 0$

shown. The imposed velocity field, which artificially ensures a homogenous simple sheared fluid field, is indicated by the dashed line. The solid particles are divided into bins according to their relative position in the y direction, and the velocity component in the flow direction, u_x , is averaged to get the data points in these plots. Despite the similarity or differences in the viscosity values and contact numbers, the averaged particle velocity profile is always very similar to the imposed fluid velocity field for both DEM and LBDEM simulations. The similarity in the averaged velocity profile indicates the capability of DEM with Stokes drag in simulating simple sheared dense suspensions, where the long-range hydrodynamic interactions are no longer necessary to obtain realistic predictions of rheology. Nevertheless, the long-range correlated dynamics of suspension, such as velocity correlation, cannot be revealed by such similarity[31].

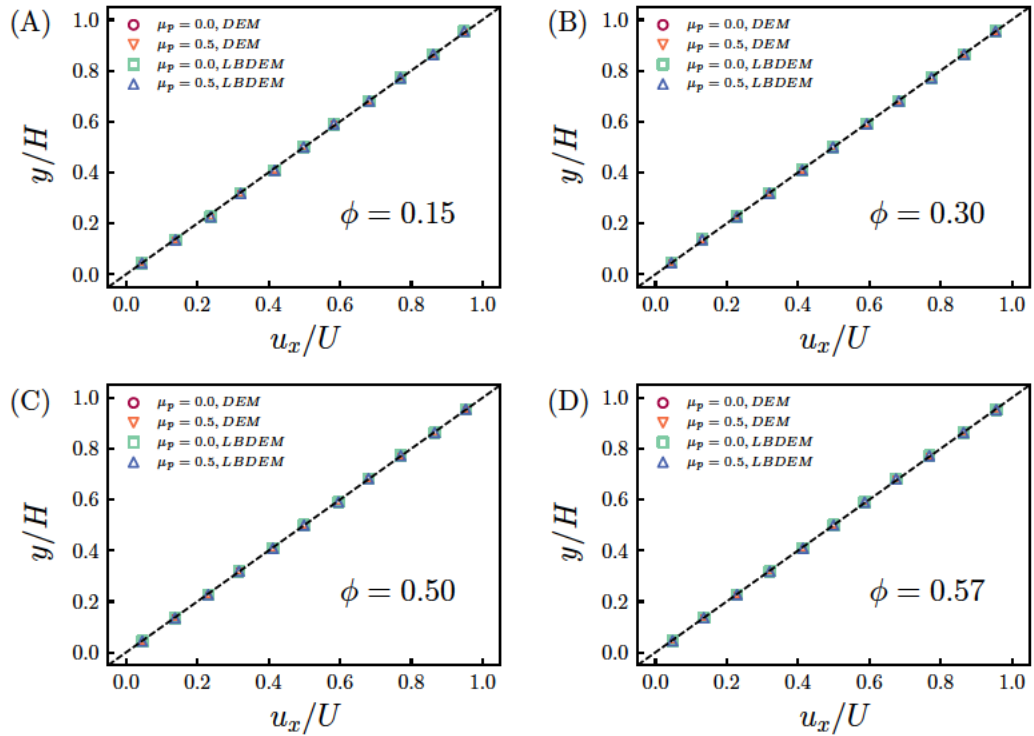


Figure 5.4 Particle velocity profiles under simple shear for different ϕ .

In this section, we compare sheared suspensions with different particle friction

coefficients ($\mu_p = 0$ or $\mu_p = 0.5$) simulated by two different approaches: the discrete element method (DEM) and the lattice Boltzmann coupled DEM (LBDEM). Our DEM approach includes the single sphere Stokes drag force (Equation(5.3)) and close-range lubrication force, while LBDEM fully resolves the fluid field. We show that both approaches produce similar viscosity results and velocity profiles in low volume fractions, where the single sphere Stokes drag force and resulting single sphere stresslet have a significant influence, as well as in high volume fractions, where particle-particle lubrication interactions and contacts dominate. However, at intermediate volume fractions, our DEM approach performs worse, as long-range hydrodynamic interactions come into play and affect the suspension rheology. We conclude that while DEM is useful for simulating low and high volume fraction behaviors, LBDEM is necessary to accurately capture the behavior of suspensions at intermediate volume fractions.

5.2.2 Frictional rheology

For the simple shear flow of dense suspensions, Boyer et al. [11] proposed a constitutive relationship to relate shear stress τ , shear rate $\dot{\gamma}$, the effective confining pressure, P^p and solid fraction ϕ as:

$$\tau = \mu(I_v) P^p \quad \text{and} \quad \phi = \phi(I_v) \quad (5.21)$$

where the macroscopic friction coefficient μ^1 and the solid volume fraction ϕ are functions of the viscous number I_v , defined as a ratio of the viscous shear stress in the fluid to the particle confining stress,

$$I_v = \frac{\eta_f \dot{\gamma}}{P^p} \quad (5.22)$$

The viscous number I_v here can be seen as the ratio between the inertial time of rearrangement $t_{\text{micro}} = \eta_f / P^p$ and the time of strain $t_{\text{macro}} = 1 / \dot{\gamma}$ [14]. When I_v is large, which means P^p is negligible compared with the viscous fluid stress, hydrodynamic interactions dominate the behaviour of the suspension, i.e. suspension is in the dilute regime. In contrast, for small I_v , short-range particle interactions dominate the suspension behaviour. The phenomenological relation

¹Note μ here is the macroscopic friction coefficient but not the particle friction coefficient μ_p .

for the friction coefficient as a function of the viscous number reads:

$$\mu(I_v) = \underbrace{\mu_1 + \frac{\mu_2 - \mu_1}{1 + I_0/I_v}}_{\mu^{\text{cont}}} + \underbrace{I_v + \frac{5}{2}\phi_m I_v^{1/2}}_{\mu^{\text{hydro}}}. \quad (5.23)$$

This relationship contains two contributions, coming from contact and hydrodynamic stresses, indicated by μ^{cont} and μ^{hydro} in the above equation. The form of the contact contribution μ^{cont} is similar to that reported for dry granular media, and the hydrodynamic contribution μ^{hydro} is designed to recover Einstein viscosity in the dilute regime. Here μ_1 , μ_2 , and I_0 are fitting parameters, as shown in Table 5.3.

Another constitutive relationship linking the solid volume fraction ϕ and the viscous number I_v reads as:

$$\phi(I_v) = \frac{\phi_m}{1 + I_v^{1/2}} \quad (5.24)$$

For a suspension sheared at a constant volume fraction, shear and normal stresses can be expressed as two functions of ϕ

$$\tau = \eta_s(\phi)\eta_f\dot{\gamma} \quad \text{and} \quad P^p = \eta_n(\phi)\eta_f\dot{\gamma} \quad (5.25)$$

where $\eta_s(\phi)$ and $\eta_n(\phi)$ are the relative shear and normal viscosities. Combining these relationships and Equation(5.23)(5.24), we can get:

$$\begin{aligned} \eta_s(\phi) &= 1 + \frac{5}{2}\phi \left(1 - \frac{\phi}{\phi_m}\right)^{-1} + \mu^c(\phi) \left(\frac{\phi}{\phi_m - \phi}\right)^2, \\ \eta_n(\phi) &= \left(\frac{\phi}{\phi_m - \phi}\right)^2, \end{aligned} \quad (5.26)$$

where $\mu^c(\phi) = \mu_1 + (\mu_2 - \mu_1) / [1 + I_0\phi^2(\phi_m - \phi)^{-2}]$. The equation above is the ϕ -dependent constitutive model for suspensions, which is aforementioned in Chapter 2.

Alternative form of $\mu(I_v)$ and $\phi(I_v)$ is adapted from the rheology of Morris and

Boulay [92] and Miller and Morris [89]:

$$\mu(I_v) = \underbrace{\mu_1}_{\mu^{\text{cont}}} + \underbrace{I_v + \frac{5}{2}\phi_m \frac{I_v^{1/2}}{K_n^{1/2}}}_{\mu^{\text{hydro}}} \quad \phi(I_v) = \frac{\phi_m}{1 + K_n^{1/2} I_v^{1/2}} \quad (5.27)$$

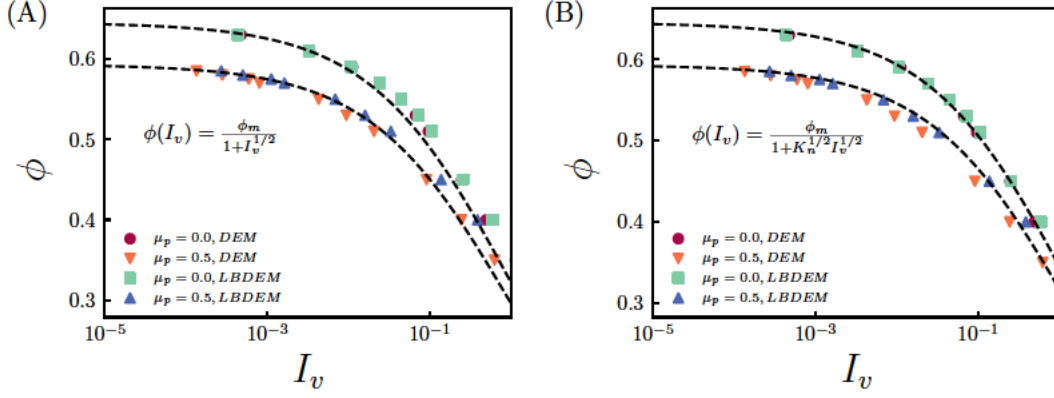


Figure 5.5 Relationship between ϕ and I_v . (A). Dashed line indicates the relationship proposed by Boyer et al. [11]. (B). Dashed line is the equation from Morris and Boulay [92]

The frictional rheology mentioned above was employed to fit our simulation results, and the $\phi - I_v$ relationship is shown in Figure 5.5. Results from DEM and LBDEM simulations are represented by scatter points, and the $\phi(I_v)$ relationships mentioned above are indicated by dashed lines. We can find that results for high volume fractions are well captured by two $\phi(I_v)$ equations with the same ϕ_m values, but Equation(5.27) provides better fitting results for high I_v , i.e. low ϕ .

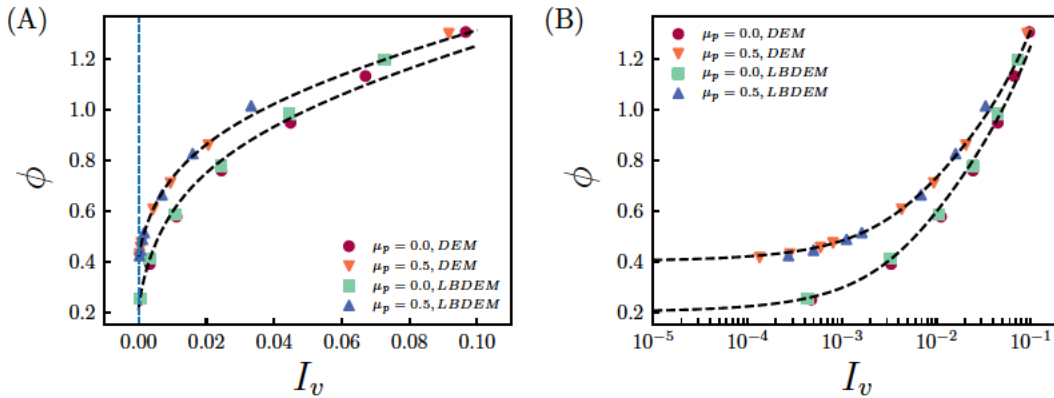


Figure 5.6 Friction coefficient $\mu = \tau/P^p$ as a function of the viscous number I_v in linear (left) and semilogarithmic (right) scales

Figure 5.5 shows the relationship between μ and I_v . The fitting equation here is

$\mu(I_v) = \mu_1 + \frac{\mu_2 - \mu_1}{1 + I_0/I_v} + I_v + \frac{5}{2}\phi_m I_v^{1/2}/K_n^{1/2}$. The fitting parameters are listed in Table 5.3.

paramters	μ_1	μ_2	I_0	K_n
$\mu = 0.5$	0.4	0.7	0.01	0.75
$\mu = 0$	0.2	0.6	0.01	0.75
Boyer et al. [11]	0.32	0.7	0.005	1

Table 5.3 *Fitting parameters for $\mu(I_v)$*

The parameters here are slightly different from Boyer et al. [11], and the fitting results indicated by blue and yellow lines only produce a good match for a low I_v regime. Despite the difference in viscosity values from different simulation approaches for $\mu_p \neq 0$ mentioned before, the simulation results from DEM and LBDEM collapse together for the $\mu - I_v$ relationship. The fitting results here also support the existence of $\mu_J^{\mu_p=0.5} = 0.4$ for frictional particles, which jam with an anisotropic microstructure at $\phi = \phi_m < \phi_{RCP}$. This μ_J is dependent on the friction coefficient of particles. Ideally, a system of frictionless particles should jam isotropically at random close particle $\phi = \phi_{RCP}$ and μ_0 . In contrast, the fitting results here suggest $\mu_J^{\mu_p=0} = 2$ for a sheared frictionless suspension, which is suspected to be caused by the broken of isotropy induced by shear. More simulations for $\phi \rightarrow \phi_{RCP}$ are warranted to verify the existence of $\mu_J^{\mu_p=0}$.

The relationships between ϕ and μ can be found in Figure 5.7. These results are for simple sheared suspensions, in which the particle distribution is homogenous. In the next chapter, an inhomogenous suspension flow will be discussed, and the $\phi - \mu$ relationship, in that case, will be compared.

5.2.3 Shear thickening behaviour

The results above are limited to the Newtonian behaviour of sheared suspensions. Here we implement a simplified electrostatic repulsion model, originally proposed by Mari et al. [86], into LBDEM to reproduce the shear thickening behaviour of suspensions.

Electrostatic repulsion model In addition to the contact force, lubrication force and hydrodynamic force, particles also experience an electrostatic repulsive force in the simulation of the solid phase, i.e. DEM part. Thus, Equation 5.1 can be

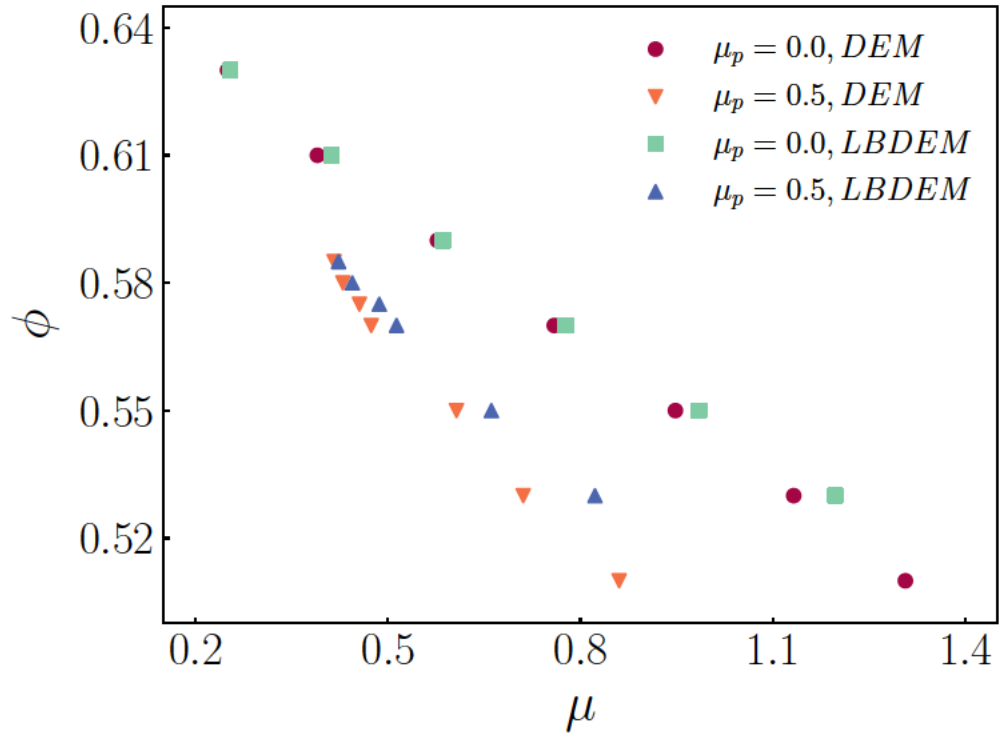


Figure 5.7 Volume fraction ϕ as a function of macroscopic friction coefficient $\mu = \tau/P^p$

rewritten as:

$$m_i \frac{d\mathbf{x}_i^2}{dt^2} = \mathbf{F}_i^C + \mathbf{F}_i^H + \mathbf{F}_i^L + \mathbf{F}_i^R \quad (5.28)$$

The repulsive force here is simplified to be a linear form, which is described as an exponential decay in Mari et al. [86], and reads as:

$$\mathbf{F}_{ij}^R \simeq \begin{cases} F^{ER}(1 - (r_{ij} - a_i - a_j)/\rho)\mathbf{n}_{ij} & \text{if } (a_i + a_j) < r_{ij} < (a_i + a_j + \rho), \\ F^{ER}\mathbf{n}_{ij} & \text{if } r_{ij} < (a_i + a_j), \end{cases} \quad (5.29)$$

where r_{ij} is the center to center distance of particle i and j . a_i and a_j are radius of particle i and j . F^{ER} is the repulsive force at contact, and ρ sets the rate of decay and the cut-off distance of the force. The repulsive force prevents particles from getting into frictional contact with a threshold force magnitude F^{ER} . The relation $F^{ER}/\rho \ll k_n$, where k_n is the spring stiffness, should be guaranteed. Otherwise, the particle radius will become artificially larger, and volume fraction ϕ have to be changed to ϕ_{eff} .

Shear-thickening behavior in suspensions is often observed by changing the shear rate in both experiments and simulations [39, 86]. Mari et al. [86] proposed a dimensionless shear rate based on the ratio between two force scales: the typical hydrodynamic force and the repulsive force F^{ER} between particles (in the critical load model discussed in Section 4.2, this force scale is denoted as F^{CL} in Equation (4.6)). Under a shear flow, the typical hydrodynamic force acting on a particle can be calculated as $6\pi\eta_f r_p U$, where U is a characteristic velocity scale and is typically expressed as $U = \dot{\gamma} r_p$ in a shear flow [36]. Based on these definitions, the characteristic shear rate and stress can be expressed as $\dot{\gamma}^* = F^{ER}/6\pi\eta_f r_p^2$ and $\sigma^* = \eta_f \dot{\gamma}^* \approx F^{ER}/6\pi r_p^2$.

Simulations of sheared suspensions require a fixed strain to reach a steady state. A lower shear rate leads to a longer simulation time for achieving the steady state, which can dramatically increase the computational cost, especially for our LBDEM method, which fully resolves the fluid field and requires many more computational sources than DEM. To address this issue and reduce computational expense, we proposed an alternative approach that employs a fixed shear rate and a tunable repulsive force F^{ER} , which results in a tunable dimensionless shear stress as well, to reproduce the shear-thickening phenomenon.

The simulation results from LBDEM simulations with ERM, shown in Figure 5.8, reproduce the increase of relative viscosity with increasing dimensionless shear

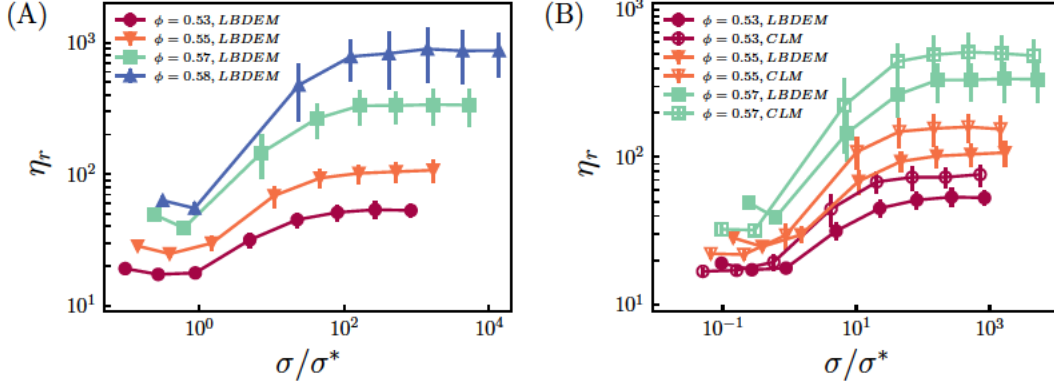


Figure 5.8 Relative viscosity as a function of non-dimensional shear stress for different volume fractions (A). Simulation results from LBDEM with ERM. (B). Comparison between LBDEM and DEM. DEM results are produced by varying shear rate $\dot{\gamma}$ with a fixed F_{CL} in CLM.

stress σ/σ^* . A shear thinning behaviour is also observed in the low σ/σ^* regime, which is observed in low $\dot{\gamma}$ regime in experiments and simulations [86]. DEM simulation results with CLM are compared in Figure 5.8(B) and provide similar viscosity values in low σ/σ^* , where the suspensions are frictionless, and higher viscosity values in high σ/σ^* , where the frictional contacts between particles are activated. The discrepancies of viscosity in the frictionless and frictional limits are consistent with Newtonian suspensions, reported in Figure 5.2.

Normal stresses Our measurements of the two normal stress differences, $N_1 \equiv \sigma_{xx} - \sigma_{yy}$ and $N_2 \equiv \sigma_{yy} - \sigma_{zz}$, are shown in Figure 5.9 and 5.10.

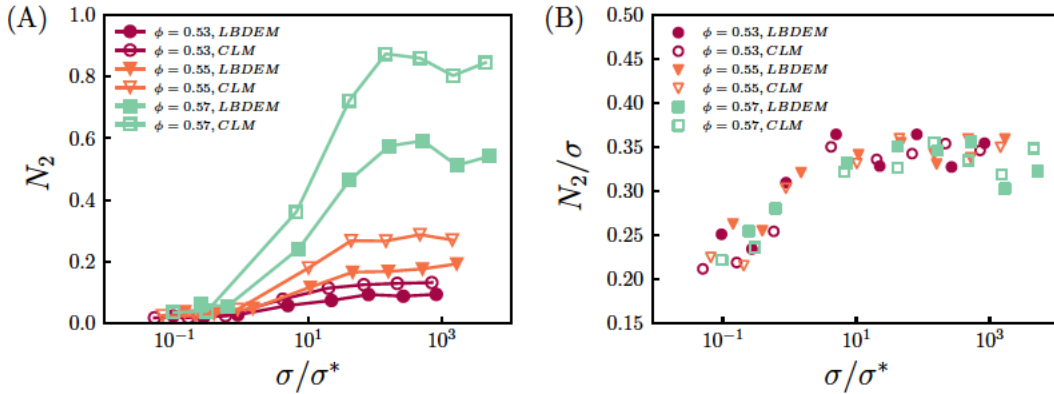


Figure 5.9 N_2 as a function of non-dimensional shear stress for different volume fractions.

We observed a negative N_2 , and the behaviour of N_2 is reminiscent of that of

the shear stress. This indicates that most of the stress is transmitted by forces in the flow gradient but not along the vorticity direction. The right plot shows that N_2/σ is not sensitive to the stress magnitude and is independent of volume fraction. All volume fractions investigated here collapse together for both ERM and CLM.

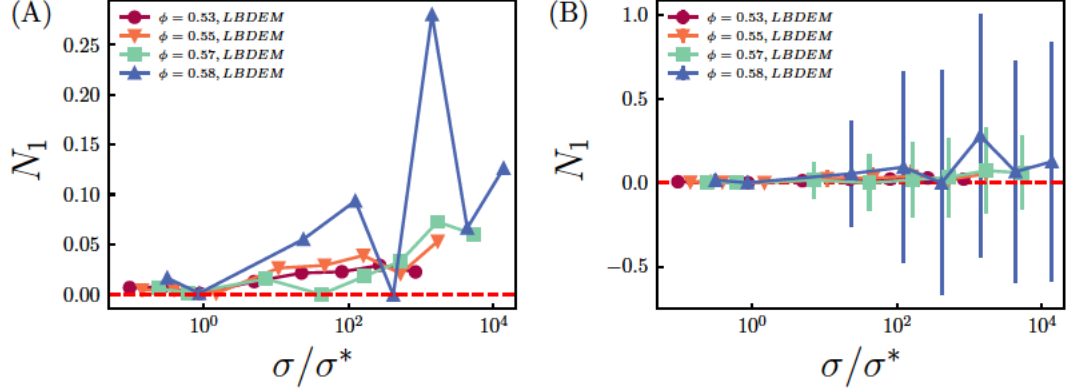


Figure 5.10 N_1 as a function of non-dimensional shear stress for different volume fractions.

The negative N_1 observed in some experiments[111] and simulations[86][7] can not be captured in our LBDEM simulations. The fluctuation of N_1 is shown in Figure 5.10(B). The fluctuation amplitude is large, compared to the average value, meaning N_1 could be either positive or negative in the time series.

5.3 Concluding Remarks

A comparison study was conducted between a coupled LBDEM approach and a DEM with short-range lubrication force for low Reynolds sheared dense suspensions with frictional and frictionless particles. Because of the lack of long-range hydrodynamic interactions, DEM produces lower viscosity than LBDEM in a semi-dilute regime, where hydrodynamic interaction dominates the rheology. For dense suspensions, where particle contacts and short-range lubrication interaction dominate, viscosity values from these two approaches are similar for frictionless particles, whereas DEM simulation produces an overestimated viscosity value than LBDEM for frictional particles. The discrepancy between these two approaches is reflected in the averaged contact number, where particle contacts are easier to generate in DEM. The physics of the discrepancies in contact numbers and viscosity values requires further investigations, considering

the velocity correlations and microstructures indicated by Gallier et al. [31].

Results from both DEM and LBDEM can be well captured by constitutive models proposed by Krieger and Dougherty [62] and Boyer et al. [11] and critical values including ϕ_J and μ_J are similar. The similarity in averaged velocity profile and $\mu-I_v$ rheology indicates that the rheology of dense suspensions under homogeneous flow can be captured by DEM with short-range lubrication force and Stokes drag.

Moreover, we proposed an alternative way to simulate the shear-thickening behaviour of dense suspensions by tuning the magnitude of the repulsive force, which is introduced to capture the transition of particle contacts from frictionless to frictional. The shear-thickening behaviour reproduced by LBDEM is comparable to existing simulation results, which support the capability of our ERM variant used in LBDEM simulations to reduce the simulation cost.

Chapter 6

Simulations of pressure driven flow of dense suspensions in a channel

In this chapter, we employ the coupled lattice Boltzmann discrete element method (LBDEM) to investigate the pressure-driven flow of dense suspensions in a square channel. We demonstrate the ability of our LBDEM method to successfully capture the shear-induced migration of solid particles and resulting particle compaction at the channel's center, which is reported by recent experiments for high solid concentration. Our method comprehensively resolves the fluid field using the lattice Boltzmann method (LBM) and captures particle-level information via the discrete element method (DEM). This allows us to directly validate the suspension balance model, which was proposed to predict the shear-induced migration, and explores the capability of frictional rheology, which is known to work well in sheared suspensions, in describing inhomogeneous suspension flow.

6.1 Introduction

6.1.1 Particle migration

Shear-induced migration is a widely encountered phenomena for suspensions, originally observed in pipe flows by Karnis et al. [57] and in channel flows by Koh et al. [61]. It describes the process that particles in suspensions migrate

irreversibly from regions of high-shear-rate to regions of low-shear-rate. In the pressure driven Poiseuille flow of suspensions, the particles migrate from the region close to the boundary towards the center, where the strain rate is close to zero. The suspension balance model (SBM), proposed by Nott and Brady [100] Nott et al. [101] Morris and Boulay [92], connects the migration flux and the pressure gradient within the solid phase and works well in describing the shear-induced migration. It is widely employed to the modelling of multiphase flow in industrial processes, such as particle separation[114], hydraulic fracture[26] and injection modeling[35].

However, recent experiments about pressure driven flow of dense suspensions with high initial volume fraction $\phi_0 = 0.55$ reported an over-compaction, where the solid volume fraction is higher the jamming volume fraction, $\phi > \phi_J$, near the center of the channel, which can not be captured by the suspension balance model.

Based on the results discussed in Chapter 5, our LBDEM simulations captures the critical behaviour of dense suspensions near jamming and provides detailed information in solid phase and fluid phase separately, which set the stage for the simulation of pressure-driven flow of dense suspensions and the investigation of SBM.

Suspension balance model

Considering a suspension consisting of non-Brownian rigid particles of density ρ_p immersed in a Newtonian incompressible fluid of density ρ_f , and viscosity η_f , we can define the local, i.e. for a specific position $\mathbf{x}$, volume fraction of the solid and fluid phase as ϕ and $1 - \phi$, respectively, and the local mean solid and fluid velocity as $\mathbf{u}^p$ and $\mathbf{u}^f$, respectively. Thus, the equations of continuity for the fluid and the particles read:

$$\frac{\partial(1 - \phi)}{\partial t} + \nabla \cdot [(1 - \phi)\mathbf{u}^f] = 0 \quad (6.1)$$

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\phi \mathbf{u}^p) = 0. \quad (6.2)$$

The incompressibility of suspension, i.e. the mixture of fluid and particles, can be described by adding Equation (6.1) and (6.2):

$$\nabla \cdot \mathbf{U} = \nabla \cdot (\phi \mathbf{u}^p + (1 - \phi) \mathbf{u}^f) = 0 \quad (6.3)$$

where $\mathbf{U}$ is the volume-averaged velocity at position $\mathbf{x}$. Combining Equation (6.3) and (6.2), the particle mass conversation equation can be rewritten as:

$$\frac{\partial \phi}{\partial t} + \mathbf{U} \cdot \nabla \phi = -\nabla \cdot \phi (\mathbf{u}^p - \mathbf{U}) \quad (6.4)$$

Here $\phi (\mathbf{u}^p - \mathbf{U})$ describes the relative motion between solid particles and the suspension, i.e. the migration flux. In the absence of inertia, the momentum balance equation $\nabla \cdot \Sigma + \rho \mathbf{g} = 0$, where Σ is the bulk average stress of suspension, of the suspension can be captured by the momentum balance of fluid and solid phases separately, which are:

$$\nabla \cdot [(1 - \phi) \langle \sigma \rangle^f + \sigma^{fp}] - n \langle \mathbf{f}^h \rangle^p + \rho_f (1 - \phi) \mathbf{g} = 0 \quad (6.5)$$

$$\nabla \cdot \sigma^{pp} + n \langle \mathbf{f}^h \rangle^p + \rho_p \phi \mathbf{g} = 0 \quad (6.6)$$

where $\mathbf{g}$ is the gravity vector. σ^{pp} is the inter-particle contact stress, which comes from particle-particle contact, and σ^{fp} is the hydrodynamic stress, which comes from the non-drag portion of the interphase interaction [77],[101],[51].

The interphase hydrodynamic force $n \langle \mathbf{f}^h \rangle^p$ in Equation (6.5) and (6.6) can be written as:

$$n \langle \mathbf{f}^h \rangle^p = -\rho_f \phi \mathbf{g} + n \langle \mathbf{f}^h \rangle_{\text{drag}}^p + n \langle \mathbf{f}^h \rangle_{\text{non-drag}}^p. \quad (6.7)$$

where three terms on the right hand side of the above equation represent the buoyancy force, the interphase drag and the non-darg part of interphase force, respectively. The interphase (fluid-solid) drag force $n \langle \mathbf{f}^h \rangle_{\text{drag}}^p$ can be approximated by a drag force proportional to the relative velocity between solid phase and fluid phase, which reads:

$$n \langle \mathbf{f}^h \rangle_{\text{drag}}^p = -\frac{18\eta_f}{d^2} \frac{\phi}{f(\phi)} (\mathbf{u}^p - \mathbf{U}), \quad (6.8)$$

where d is the particle diameter and $f(\phi)$ is the empirical hindered settling function and has different forms as shown in Table 6.1. Figure 6.1 taken from Lecampion and Garagash [75] shows different expressions for the hindered equations and related results from experiments and simulations.

We can then rewrite Equation (6.6) as:

$$\nabla \cdot \boldsymbol{\sigma}^p + n \langle \mathbf{f}^h \rangle_{drag}^p + (\rho_p - \rho_f) \phi \mathbf{g} = 0 \quad (6.9)$$

where $\boldsymbol{\sigma}^p = \boldsymbol{\sigma}^{pp} + \boldsymbol{\sigma}^{hp}$. The buoyancy force term $(\rho_p - \rho_f) \phi \mathbf{g}$ can be neglected for neutrally buoyant particles ($\rho = \rho_p = \rho_f$). Thus we can get:

$$\phi (\mathbf{u}^p - \mathbf{U}) = \frac{d^2 f(\phi)}{18\eta_f} \nabla \cdot \boldsymbol{\sigma}^p \quad (6.10)$$

From the suspension balance model, we can expect that particle migration is driven by the divergence of the normal components of the particle phase stress $\boldsymbol{\sigma}^p = \boldsymbol{\sigma}^{pp} + \boldsymbol{\sigma}^{hp}$.

Reference	Equation
Carmen-Kozeny[46]	$0.1(1 - \phi)^3 \phi^{-1}$
Richardson-Zaki ⁴⁴ [130]	$(1 - \phi)^n$
van der Hoef[130]	$[(1 - \phi)(1 - 1.5\sqrt{\phi}) + 10\phi(1 - \phi)^{-3}]^{-1}$
Mills and Snabre[90]	$(1 - \phi) [1 + 4.6\phi(1 - \phi)^3]^{-1}$
Effective medium theory[43] [140]	$(1 - \phi)^2(1 - \tilde{\phi})^2$

Table 6.1 *Closure relations for hindered settling function $f(\phi)$ of monodisperse suspension. Here $\tilde{\phi} = \phi/\phi_{\max}$. Table is taken from Vollebregt et al. [131]*

As mentioned in Section 3.3.3, the migration flux $\phi (\mathbf{u}^p - \mathbf{U})$ can be calculated by averaging the lattice information (velocity components v_x, v_y, v_z and solid fraction ϵ) from LBM and the divergence of the particle phase stress $\boldsymbol{\sigma}^p$ can be calculated by averaging particle level information from DEM.

6.2 Methodology

Details about the coupled lattice Boltzmann discrete element method (LBDEM) has been introduced in Chapter 3 and summarised in Chapter 5. Here we provide details about the simulation setup of our channel flow.

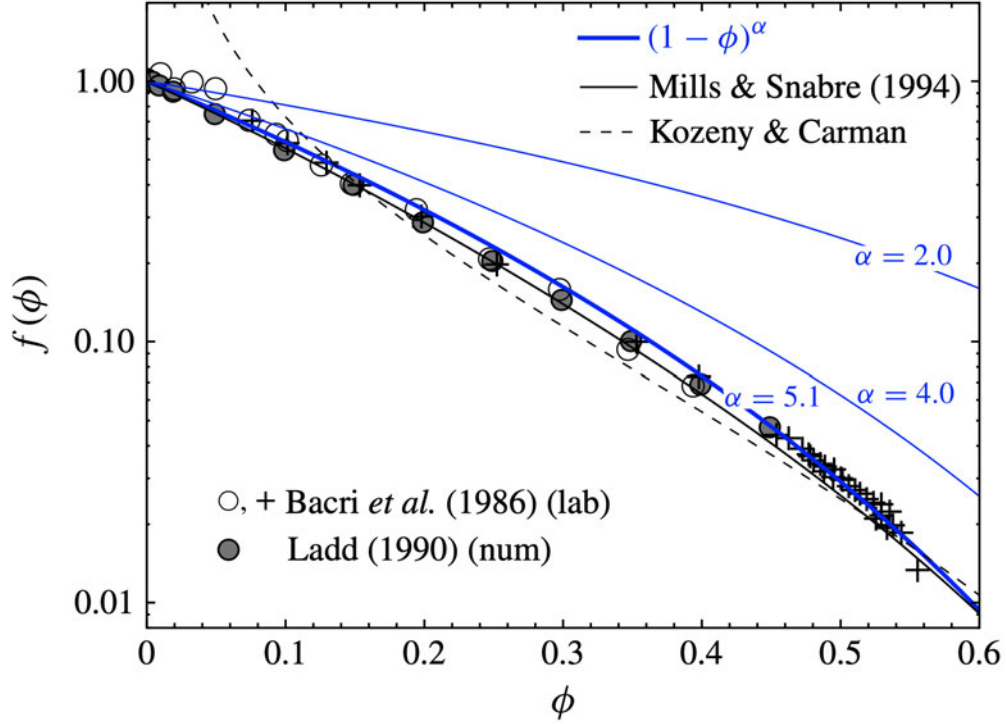


Figure 6.1 Different phenomenological expressions for the hindrance function $f(\phi)$ in log-linear scale (with the corresponding normalized permeability function given by $\kappa(\phi) = 2f(\phi)/9\phi$) are contrasted with the data from batch sedimentation experiments (Bacri et al. [4]), and from the numerical simulations of the dispersion of hard spheres (Ladd and Frenkel [68]). The Richardson & Zaki empirical form, $f = (1 - \phi)^\alpha$ with $\alpha = 5.1$ (Garside & Al-Dibouni 1977; Davis & Acrivos 1985), and Mills & Snabre [90] theoretical expression, $f = (1 - \phi)/(1 + 4.6\phi/(1 - \phi)^3)$, are in excellent agreement with both the experimental and numerical data over the entire (flowing) range of the solid volume fraction. Kozeny-Carman's expression [46], $f = (1 - \phi)^3/10\phi$, provides an adequate approximation of the sedimentation data for all but dilute ($\phi \lesssim 0.1$) suspensions. Both the figure and the caption are taken from Lecampion and Garagash [75]

6.2.1 Simulation setup

In this work, pressure driven flows of suspensions in a square channel are simulated by LB-DEM coupling. The simulation domain size is fixed as $40d_p \times 20d_p \times 20d_p$, where d is the particle diameter. The flow direction (x) is periodic and the boundaries in y and z direction are solid walls, as shown in Figure 6.2. Details about the boundary conditions are discussed in the section below.

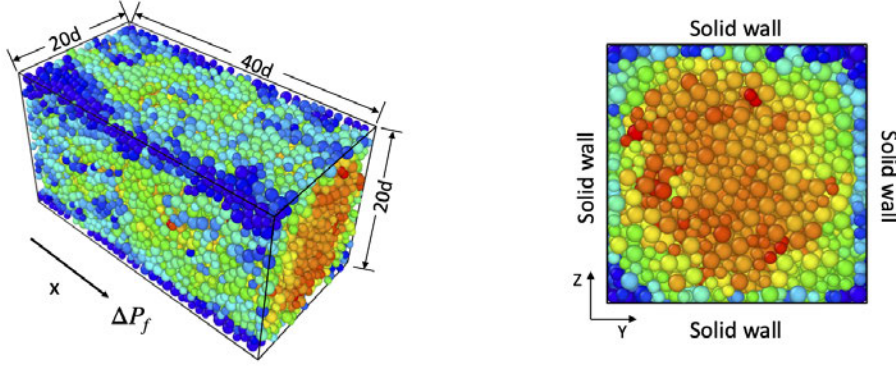


Figure 6.2 Snapshots of the simulated channel flow. Colors represent the particle velocity. The size of the channel is $40d_p \times 20d_p \times 20d_p$ with periodic boundary in flow direction, which is x direction here and solid walls in xz and xy plane.

Boundary conditions for the square channel

Periodic Boundary Conditions with Pressure Variations In our LBD-DEM simulation of pressure-driven flow, a periodic boundary condition with pressure variations in LBM, proposed by Kim and Pitsch [59] and named as the generalized periodic boundary condition (GPBC), is employed in the flow direction.

The generalized periodic boundary condition assumes that the simulation system is periodic with an additional prescribed pressure drop Δp along the flow direction. In an isothermal fluid, The fluid density and pressure are related in an isothermal fluid, i.e. $p = c_s^2 \rho$, which means the pressure drop can be achieved in a density drop between inlet and outlet of the channel. Thus, for incompressible flows, the generalized periodic boundary condition reads:

$$\begin{aligned} p(\mathbf{x}) &= p(\mathbf{x} + \mathbf{L}) + \Delta p \\ \mathbf{u}(\mathbf{x}, t) &= \mathbf{u}(\mathbf{x} + \mathbf{L}, t) \end{aligned} \quad (6.11)$$

where Δp is a prescribed variation of the pressure.

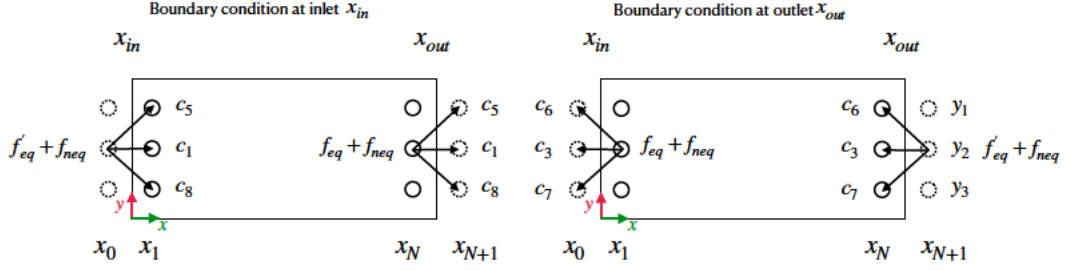


Figure 6.3 Sketch of the generalized periodic boundary condition in LBM. Layers of "virtual" nodes, denoted by dashed circles, are added before and after the periodic boundaries, i.e. at $x_0 = x_1 - \Delta x$ and $x_{N+1} = x_N + \Delta x$, respectively. Figure is adapted from Kim and Pitsch [59]

As shown in Figure 6.3, two layers of "virtual nodes" are added before and after the periodic boundary, and the particle distribution function on these virtual nodes can be decomposed into equilibrium parts f^{eq} and non-equilibrium parts f^{neq} , i.e. $f^* = f^{eq} + f^{neq}$, where f^* denotes the particle distribution function after collision. For satisfying Equation(6.11), the equilibrium part should be written as:

$$\begin{aligned} f_i^{eq}(x_0, y, t) &= f_i^{eq}(p_{in}, \mathbf{u}_N) \\ f_i^{eq}(x_{N+1}, y, t) &= f_i^{eq}(p_{out}, \mathbf{u}_1) \end{aligned} \quad (6.12)$$

where $\mathbf{u}_N$ and $\mathbf{u}_1$ are, respectively, the velocity at nodes x_N and x_1 . p_{in} and p_{out} are the pressure values at the inlet and outlet. The pressure drop $\Delta p = p_{in} - p_{out}$ describes the pressure difference between inlet and outlet boundaries and influences the fluid velocity and the Reynolds number (Re) of the simulation.

The non-equilibrium part is copied from the corresponding image points inside the real domain, i.e.

$$\begin{aligned} f_i^{neq}(x_0, y, t) &= f_i^{neq}(x_N, y, t), \\ f_i^{neq}(x_{N+1}, y, t) &= f_i^{neq}(x_1, y, t). \end{aligned} \quad (6.13)$$

As a conclusion, the particle distribution function at the boundaries are:

Inlet boundaries:

$$f_i^*(x_0, y, t) = f_i^{eq}(p_{in}, \mathbf{u}_N) + (f_i^*(x_N, y, t) - f_i^{eq}(x_N, y, t)) \quad (6.14)$$

Outlet boundaries:

$$f_i^*(x_0, y, t) = f_i^{\text{eq}}(p_{\text{in}}, \mathbf{u}_N) + (f_i^*(x_N, y, t) - f_i^{\text{eq}}(x_N, y, t)) \quad (6.15)$$

and the pressure drop assigned in the simulation is $\Delta p = p_{\text{in}} - p_{\text{out}}$.

The periodic boundary in DEM means that particles can interact across the boundary, and they can exit one boundary of the box and re-enter the other one along the periodic direction.

Solid walls Besides the flow direction x , boundaries in other two directions are set as solid wall boundaries. The wall boundaries have the same friction coefficients and spring constant as solid particles for the solid phase in DEM. A no-slip boundary condition, non-equilibrium bounce-back method (NEBB) or named as Zou-He method introduced in Section 3.2.4, is used in LBM part. Here the lubrication effect between solid walls and particles is ignored as a careful calibration and implementation of lubrication between wall and particles are complex, especially in the corner of the channel, and the inter-particle contact is the stress dominating contribution for dense suspensions[94].

Initial states

In this work, we have simulated 6 different cases with different volume fractions and friction coefficients, as listed in Table 6.2.

ϕ_0	0.4	0.4	0.5	0.5	0.55	0.55
μ_p	0	0.5	0	0.5	0	0.5

Table 6.2 *Summary of simulation cases studied*

With a given solid fraction ϕ_0 , a corresponding number of bi-disperse rigid spheres at particle diameters 1d and 1.4d (to prevent crystallization) are mixed in equal volume and distributed homogeneously in the simulation domain, which means the initial state of our simulations have a homogeneous solid volume fraction profile. For the LBM part, the initial state is to set initial particle distribution functions to equilibrium, i.e. $f_i(\mathbf{x}, t = 0) = f_i^{\text{eq}}(\rho(\mathbf{x}, t = 0), \mathbf{u}(\mathbf{x}, t = 0))$. In this work, the initial velocity field is $\mathbf{u}(\mathbf{x}, t = 0) = \mathbf{0}$ and the pressure/density field has a pressure gradient($\Delta\rho/L$), where L is the channel size in flow direction.

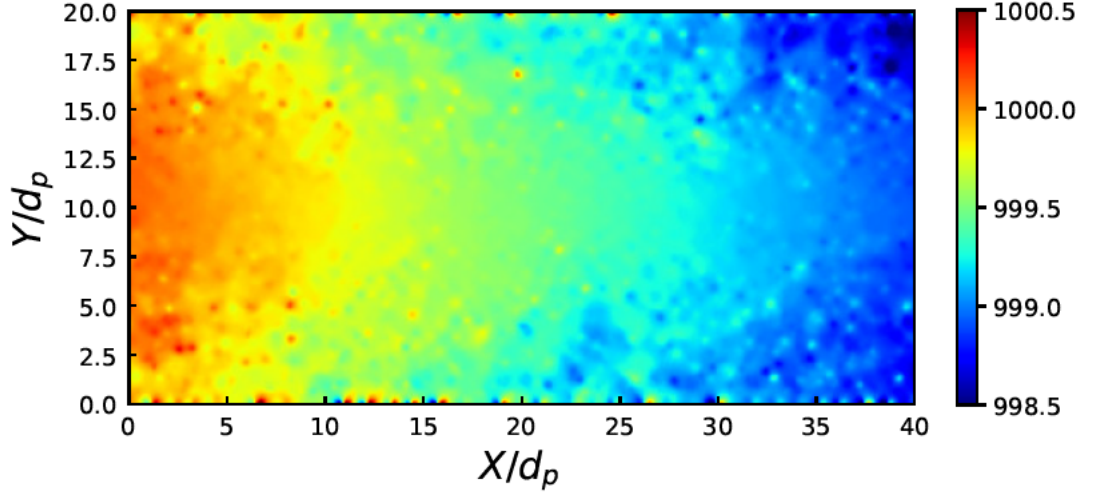


Figure 6.4 Snapshot of the distribution of density values in each lattice (SI units kg/m^3) in X-Y plane.

Simulation parameters

In our simulation, we set the solid particle diameter d_p and density ρ_p as 0.0005 m and 1000 kg/m^3 , respectively. The fluid density ρ_f , kinematic viscosity ν_f and dynamic viscosity η_f are 1000 kg/m^3 , $10^{-4} \text{ m}^2/\text{s}$ and 0.1 $\text{Pa} \cdot \text{s}$ respectively. With the collision relaxation parameter set as 0.65, the simulation time step of LBM can be calculated from Equation(5.12): $\Delta t_{LBM} = 1.25 \times 10^{-6} \text{ s}$. Thus, the simulation time step of DEM Δt_{DEM} is $2.5 \times 10^{-8} \text{ s}$ as 50 DEM time steps are performed between two sequential LBM timesteps, i.e. $\Delta t_{LBM} = 50 \Delta t_{DEM}$. The spring stiffness k_n and damping coefficient γ_n of hooke model in DEM are set as 10500 N/m and 3000 kg/s, which satisfy the relation $\gamma_n = 2/7 k_n$ proposed by Schäfer et al. [116].

The pressure difference between inlet and outlet of the channel is accomplished by setting a density difference $\Delta \rho = \Delta P / c_s^2$, where c_s is the sound speed. As shown in Figure 6.4, the density generally decreases from the inlet to the outlet boundary of the channel, and the maximum density difference is no more than 2

kg/m³. The density difference is much smaller than the particle density, and the neutrally buoyancy holds in our simulation. Here the particle Reynolds number is calculated based on the definition proposed by Lyon and Leal [84], $Re_{p,LL} = 2\rho d_p^3 \langle u \rangle / (3\eta_f H^2)$. The averaged particle velocity, calculated from the simulation results as shown in Figure 6.10, varies from 0.003 m/s to 0.3 m/s. The range of the particle Reynolds number in our simulations is $0.002 \sim 0.02$, where the inertia effect is negligible. For further discussion, we proposed the characteristic velocity and timescale as $u_c = d_p / (\eta_f / \Delta p)$ and $t_c = \eta_f / \Delta p$.

6.2.2 Post-processing

To coarse-grain the simulation results for obtaining pseudo-continuous data, particles inside a sub channel with bin size [4d, 4d, 40d] are averaged. As illustrated in Figure 6.5, the averaged particle velocity of the center of black box shown in left-hand figure is calculated by averaging over particles shown in the right-hand figure, i.e.

$$\mathbf{u}^p = \frac{\sum_{\text{particles}} \mathbf{u}_i^p}{N_{\text{particles}}} \quad (6.16)$$

Other particle-level information like Voronoi volume fraction ϕ_{voro}^1 and stress components σ_{ij} can be calculated in this way as well.

Simulation results of fluid phase can be obtained from each lattice node in LBM, which has finer resolution than particles as $\Delta x = 0.1d_p$. As mentioned before, the solid fraction ϵ of each lattice can be calculated by the sub-grid method in PSM. Thus the average of solid phase information and fluid phase information can be calculated separately with the given solid fraction. For example, the averaged solid phase velocity and fluid phase velocity can be calculated by:

$$\mathbf{u}^s = \frac{\sum_{\text{lattices}} \mathbf{u}_i^l \phi_s^l}{\sum_{\text{lattices}} \phi_s^l} \quad (6.17)$$

$$\mathbf{u}^f = \frac{\sum_{\text{lattices}} \mathbf{u}_i^l (1 - \phi_s^l)}{\sum_{\text{lattices}} (1 - \phi_s^l)} \quad (6.18)$$

¹The Voronoi volume fraction refers to the ratio of the volume of the Voronoi cells to the total system volume. Voronoi cells are regions of space defined by the perpendicular bisectors of the lines connecting adjacent particle centers. The boundaries of the cells correspond to planes equidistant to neighboring particle centers, and the cells are convex polyhedra that fully partition the space. By calculating the volume of these cells, one can determine the amount of space that is void of any particles in a suspension system. This is useful for characterizing particle packing and identifying regions of low or high particle density within a suspension.

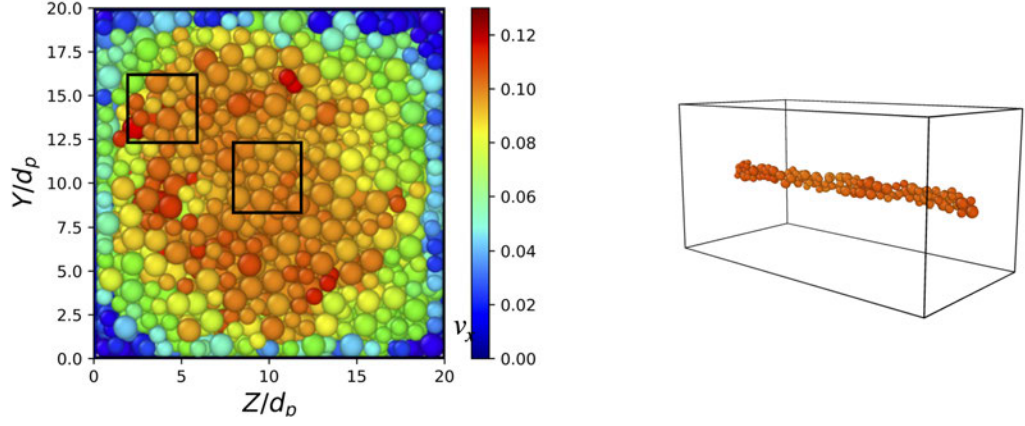


Figure 6.5 Sketch of post-processing for solid phase. Left-hand figure is a snapshot of DEM results. The color of solid particles are assigned by their velocity values in flow direction (u_x). Right-hand figure shows the solid particles inside one given bin in the simulation box.

$$\mathbf{U} = \frac{\sum_{\text{lattices}} \mathbf{u}_i^l}{N_{\text{lattices}}} \quad (6.19)$$

where ϕ_s is the solid fraction value in the lattice, $\phi_s = \epsilon$.

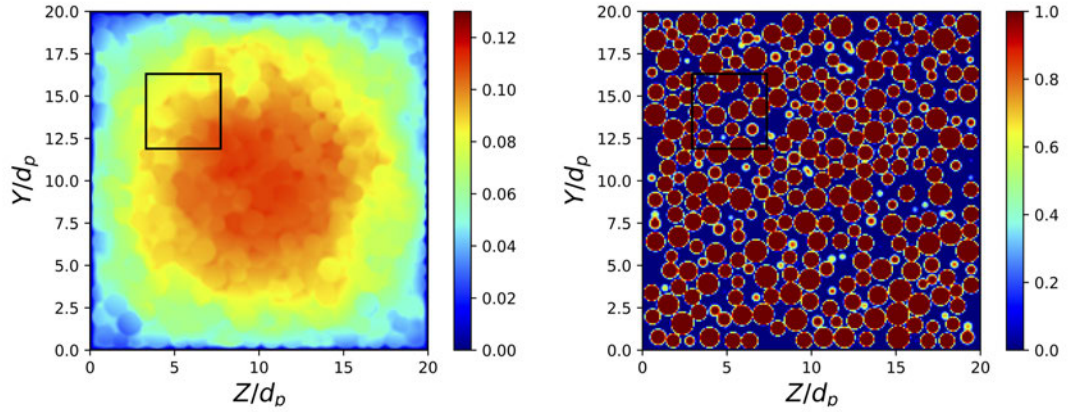


Figure 6.6 Snapshots of simulation results in Y-Z plane for fluid phase. Left-hand figure shows u_x of each lattice with SI unit (m/s). Right-hand figure shows the solid fraction ϵ calculated from PSM in each lattice.

6.3 Results

6.3.1 Particle Migration in the channel

In this section, we present the time evolution of the velocity profile of the suspension as well as the solid volume fraction, which is measured by the averaged voronoi volume fraction ϕ_{voroi} of solid particles here, for different volume fractions and friction coefficients as listed in Table 6.2.

Shear-induced migration By averaging over the cross-section of the channel, we can get the distribution of ϕ_{voroi} and $u_x/\langle u_x \rangle$, as shown in Figure 6.8 and 6.7 at a specific simulation time t/t_c . It is obvious that ϕ_{voroi} and the shear rate, defined as the velocity gradient, $\Delta u_x/\Delta x$, of neighbour bins, are lower in the center than the edge of the square channel, which reflects the migration of particles from the edge, where shear rate is high, to the center, where shear rate is low. Thus, the shear-induced migration is successfully captured by our simulations. The distribution of u_x and ϕ_{voroi} is influenced by ϕ_0 and μ_p . A much wider blunted velocity profile is observed for denser frictional suspensions. Similar trend can also be observed in ϕ_{voroi} profile.

Overcompaction Furthermore, we also observe that ϕ_{voroi} reaches a maximum constant value of about 0.63 ($> \phi_J^{\mu_p=0.5} \approx 0.593$) in a finite subregion within the blunted velocity profile, which is defined as a jammed domain[102] where the macroscopic shear rate $\Delta u_x/\Delta x$ is close to 0, for both frictional suspensions and frictionless suspensions. Thus, an evident over-compaction[102][75][32], where $\phi > \phi_J$, is also simulated in the pressure driven flow of dense suspensions.

Travel length and entrance length For measuring the time required for a pressure driven suspension flow in the channel to reach a fully developed steady state, a transition length, or entrance length, was proposed by Nott and Brady [100] and reads:

$$L_{ENT} \propto H^3/d_p^2 \quad (6.20)$$

where H is the height of the channel, or diameter of the pipe, and d_p is the particle diameter. In our simulation system, L_{ENT} is estimated to be $8000d_p$, given that $H/d_p = 20$. The entrance length is also influenced by the entrance volume

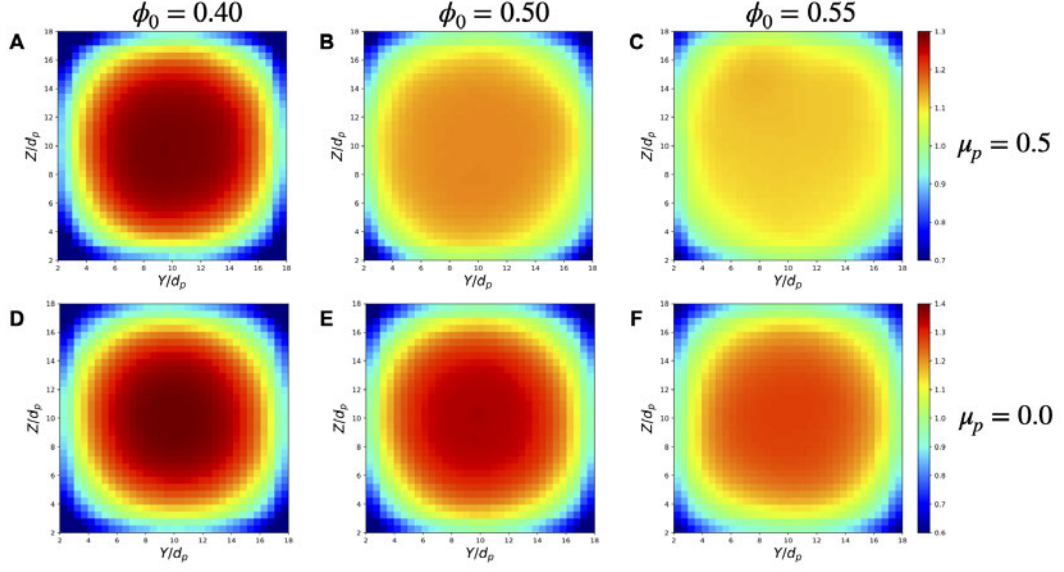


Figure 6.7 The averaged velocity $u_x/\langle u_x \rangle$ field in the Y-Z plane of the channel. (A) $\phi_0 = 0.4$ and $\mu_p = 0.5$ at $t/t_c = 524$. (B) $\phi_0 = 0.5$ and $\mu_p = 0.5$ at $t/t_c = 633$. (C) $\phi_0 = 0.55$ and $\mu_p = 0.5$ at $t/t_c = 672$. (D) $\phi_0 = 0.4$ and $\mu_p = 0$ at $t/t_c = 524$. (E) $\phi_0 = 0.5$ and $\mu_p = 0$ at $t/t_c = 633$. (F) $\phi_0 = 0.55$ and $\mu_p = 0$ at $t/t_c = 672$.

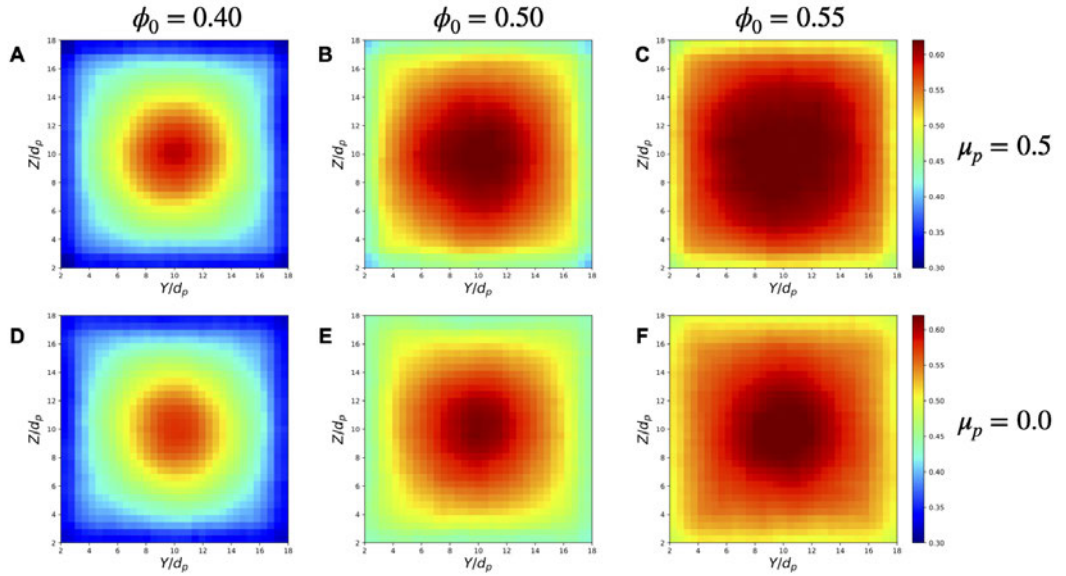


Figure 6.8 The averaged voronoi volume fraction ϕ_{voro} field in the Y-Z plane of the channel.

fraction ϕ_0 according to Lecampion and Garagash [75]. For example, the L_{ENT} is estimated as $0.05H^3/d_p^2$ and $0.01H^3/d_p^2$ for $\phi_0 = 0.5$ and 0.55 , respectively[102].

The travel length of the suspension is estimated by an accumulative length, defined as:

$$L_{travel}(t) = \sum_i \langle u_{x,i} \rangle \Delta t \quad (6.21)$$

where $\langle u_{x,i} \rangle$ is the average velocity during time period $[t_i, t_i + \Delta t]$. With the development of $\langle u_x \rangle$ provided in Figure 6.10, we find that the travel lengths, L_{travel} , in our simulation are close to the estimated L_{ENT} for $\phi_0 = 0.5$ and $\phi_0 = 0.55$, which means our simulations have reached, at least close to, the fully developed state. Our discussion below focuses on $\phi_0 = 0.5$ and $\phi_0 = 0.55$ since the travel length for $\phi_0 = 0.4$ is smaller than the estimated entrance length $L_{ENT}^{\phi_0=0.4}$ and the over-compaction is not obvious in this case.

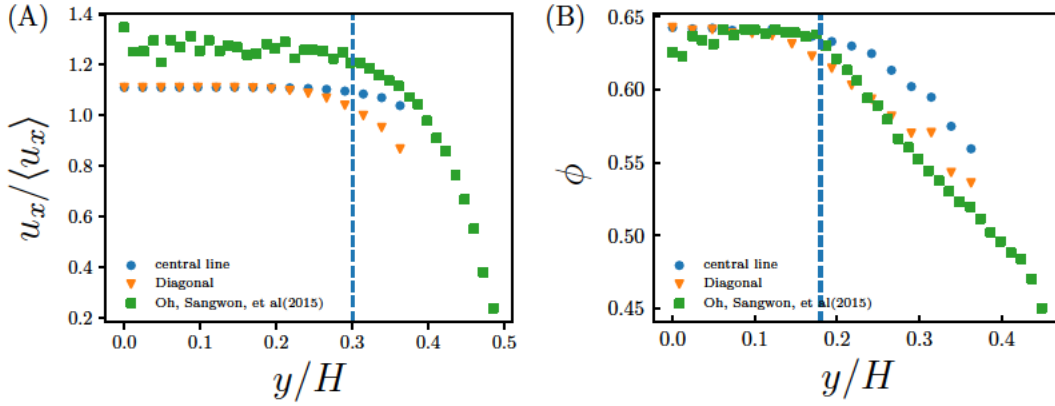


Figure 6.9 The (A) u_x and (B) ϕ at $t/t_c \approx 720$ are shown for $\phi_0 = 0.55$. Results are taken from the central line, where $y = 0.5H$ or $z = 0.5H$, and the diagonal line of the cross-section of the channel. Experimental results taken from Oh et al. [102] are shown as diamonds and the estimated width of the jammed region, and central plug from Oh et al. [102] are indicated by dashed vertical lines.

The boundary effect of the solid wall on the velocity profile is not negligible for a square channel with channel width $D = 20d_p$. Thus we can only compare our simulation results with experimental results qualitatively, as shown in Figure 6.9. Results taken from the central line and diagonal line of snapshots at $t/t_c \approx 720$, where the suspension is considered as fully developed with a travel length estimation, for $\phi_0 = 0.55, \mu_p = 0.5$, are compared with experimental results of the pressure-driven suspension flow ($\phi_0 = 0.55$) in a pipe[102]. Oh et al. [102] defined a jammed region according to the velocity profile, where the velocity is lower than the maximum value by an arbitrary small fraction (1% in the experiments),

and a central plug, where ϕ reaches a maximum constant value of 0.64 ($\approx \phi_{RCP}$) in a finite subregion within the jammed material domain. The width of the jammed region and central plug are $0.3H$ and $0.18H$ for $\phi_0 = 0.55$, which are indicated by dashed vertical lines in Figure 6.9. Due to the wall boundary effect, our simulation results are slightly different between central line and diagonal line. Thus we define the jammed region and central plug by the area where $u_x > 0.99u_x^{max}$ and $\phi_{voro} > 0.99\phi_{voro}^{max}$, respectively. The evolution of $\langle V_x \rangle$, ϕ_{voro}^{max} and the normalized area (S/S_{square}) of jammed region and central plug can be found in Figure 6.10. The development of V_x is faster than ϕ [75][84], and the fluctuation of jammed region and central plug, especially for $\mu_p = 0.5$, can not be neglected[50]. The estimated normalized area of jammed region and central plug for $\phi_0 = 0.55, \mu_p = 0.5$ are 0.36 and 0.14, respectively, which are similar to the experimental results by Oh et al. [102].

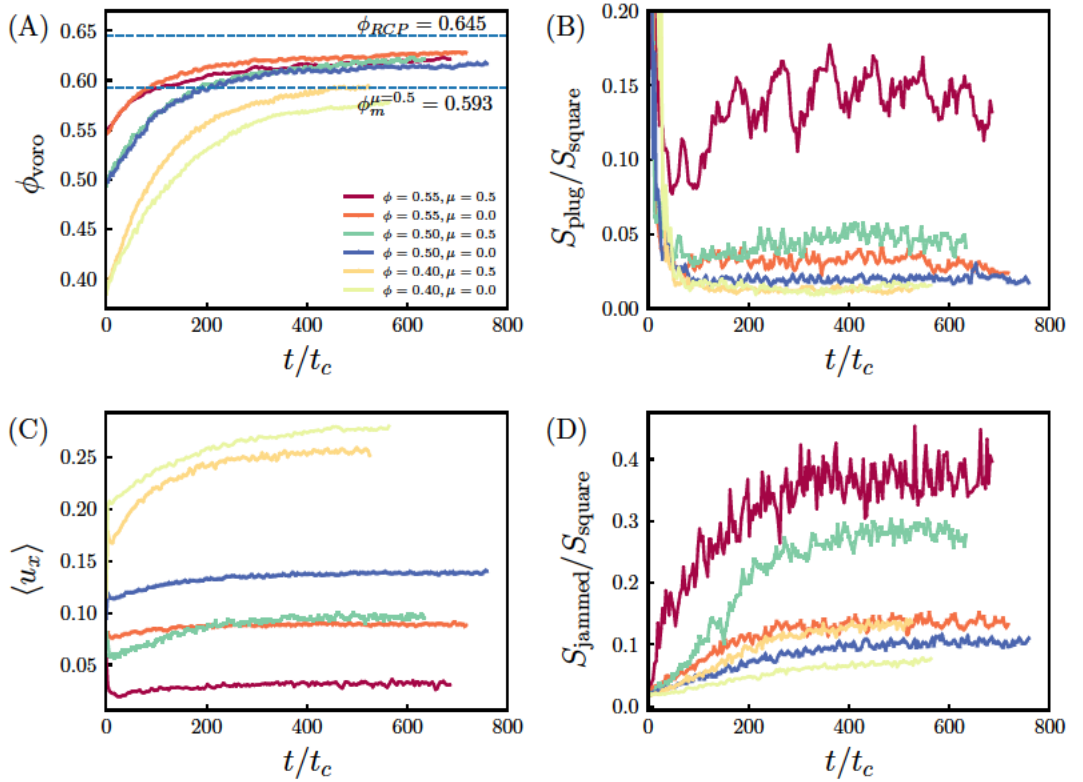


Figure 6.10 (A) Evolution of maximum ϕ_{voro} . $\phi_J^{\mu=0.5}$ and ϕ_{RCP} from Chapter 5 are indicated by red dashed lines. (B) Evolution of the normalized area of the central plug, where $\phi_{voro} > 0.99\phi_{voro}^{max}$. (C) Evolution of the averaged velocity $\langle u_x \rangle$. (D) Evolution of the normalized area of the jammed region, where $u_x > 0.99u_x^{max}$.

According to the discussion above, our LBDEM simulations of pressure driven flow successfully capture the shear-induced migration in the channel and the over-

compaction, where $\phi > \phi_J$ for frictional particles, in the center of the channel. Subtracting the results of the central line ($y/H = 0.5$) of each snapshot (Figure 6.8) output from simulations, we can get the time evolution, i.e. the transient dynamics of the migration process of ϕ_{voro} for different ϕ_0 and μ_p , which has never been reported yet.

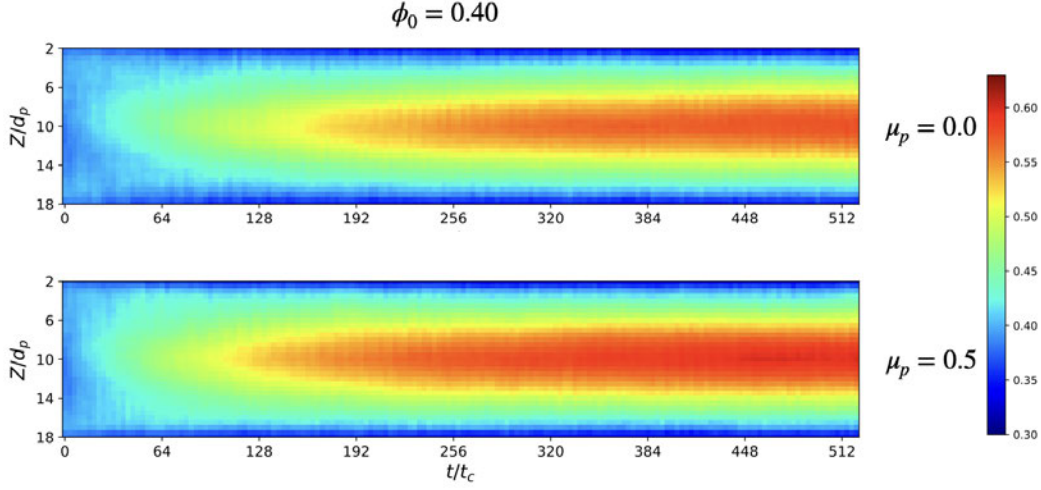


Figure 6.11 The time evolution of the voronoi volume fraction ϕ_{voro} for $\phi_0 = 0.4$

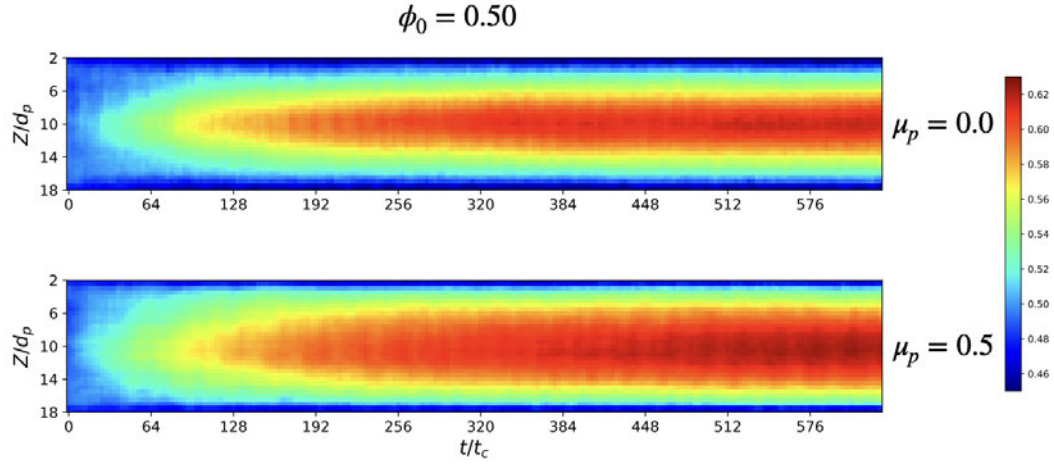


Figure 6.12 The time evolution of the voronoi volume fraction ϕ_{voro} for $\phi_0 = 0.5$

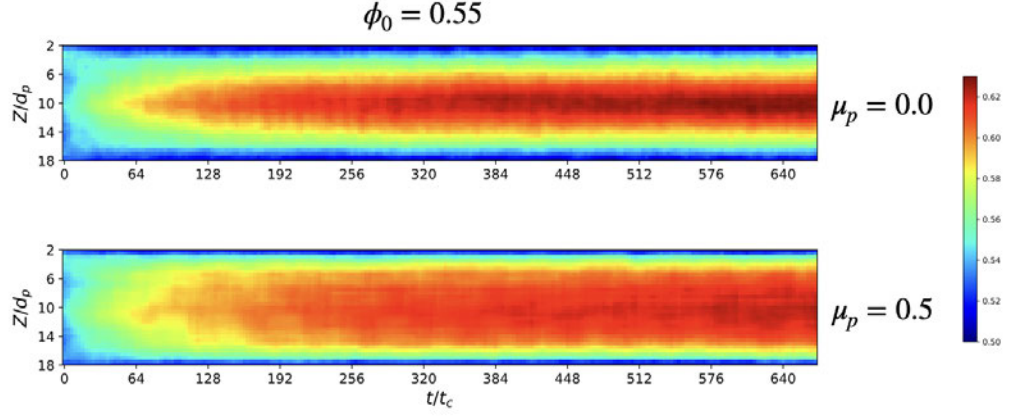


Figure 6.13 The time evolution of the voronoi volume fraction ϕ_{voro} for $\phi_0 = 0.55$

6.3.2 Comparison with the suspension balance model

With a proper post-processing of lattice-level information from LBM and particle-level information from DEM, we can get the migration flux, left side of Equation 6.10 and the gradient of normal stress component, right side of Equation 6.10, as shown in Figure 6.14. We find that the trend of velocity difference ($U_y - u_y^s$) and pressure gradient $\nabla_y \sigma_{yy}$ are the same for both frictional and frictionless suspensions at $t/t_c = 30$, which indicates the governing equation (Equation 6.10) of suspension balance model holds.

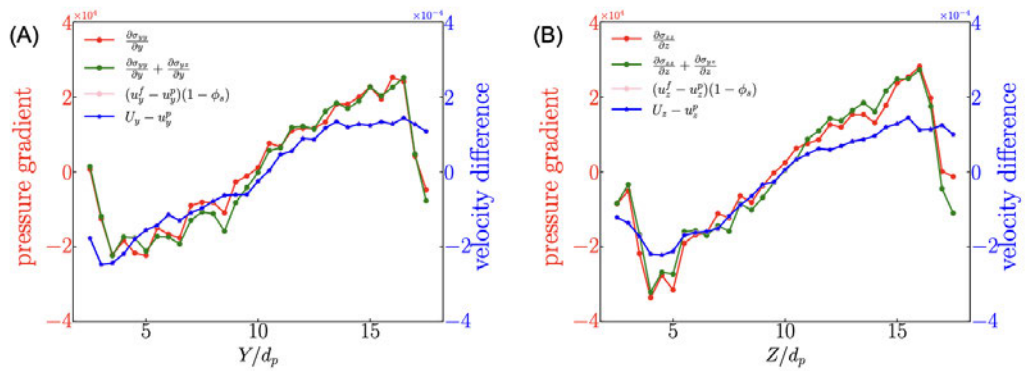


Figure 6.14 Y-direction components of pressure gradient and velocity difference as a function of Y/d_p . (A) $\phi_0 = 0.55, \mu_p = 0$ at $t/t_c = 30$. (B) $\phi_0 = 0.55, \mu_p = 0.5$ at $t/t_c = 30$. Results here are taken from cubic bins in the central line ($y=H/2$).

Figure 6.15 shows the fitting results of different hindered functions $f(\phi)$. Here we choose $n = 5$, following Guazzelli and Pouliquen [37] for Richardson-Zaki(R-Z) function: $(1 - \phi)^n$. Each scatter point represents the averaged results from each cubic bin as discussed in the post-processing section. A linear regression analysis over these scatter points are conducted through a popular Python package: statsmodels and related fitting results are reflected by the slope of the dashed line in Figure 6.15. The fitting result are the same for different hindrance functions but differ for different friction coefficients. Moreover, the dependence between migration flux and pressure gradient is not valid at $t/t_c = 300$ (Figure 6.16), where the suspension is “partially” developed, as shown in Figure 6.13.

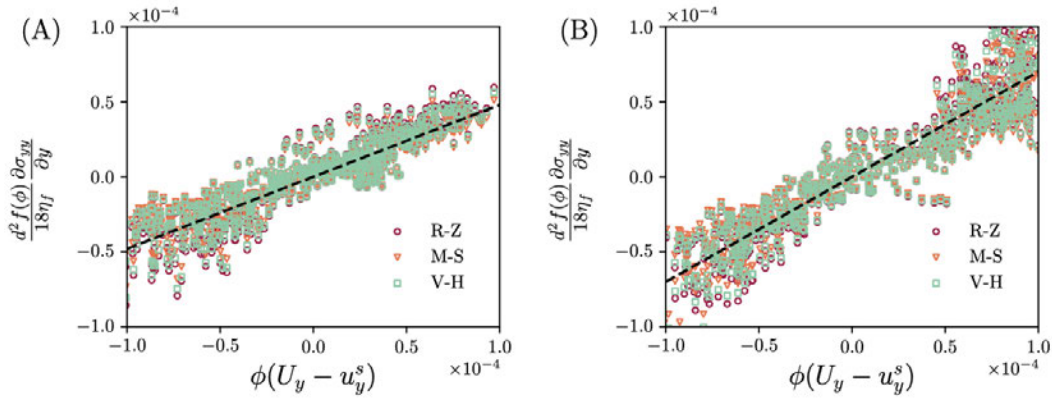


Figure 6.15 Test of hindered functions $f(\phi)$ listed in Table 6.1 at $t/t_c = 30$. (A) $\mu_p = 0$ and the slope of the dashed black line is 0.5. (B) $\mu_p = 0.5$ and the slope of the dashed black line is 0.7.

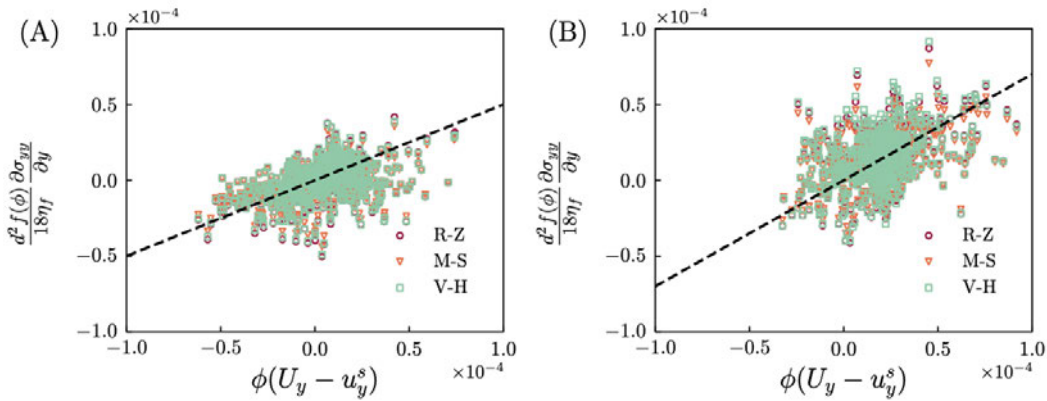


Figure 6.16 The relationship between pressure gradient and migration flux at $t/t_c = 300$.

To figure out the difference between suspensions at $t/t_c = 30$ and $t/t_c = 300$, we compare the distribution of ϕ , u_x and $\dot{\gamma}_{square}$ (Figure 6.17). Here we define the shear rate $\dot{\gamma}_{square}$ as: $\dot{\gamma}_{square} = \sqrt{\dot{\gamma}_{xy}^2 + \dot{\gamma}_{xz}^2}$. Similarly, shear stress τ_{square} can be defined as $\tau_{square} = \sqrt{\tau_{xy}^2 + \tau_{xz}^2}$.

Compared to the suspension at $t/t_c = 30$, the suspension at $t/t_c = 300$ shows a clear central plug zone, where $\phi \rightarrow \phi_{RCP} = 0.64$ and jammed region, where the velocity profile is blunted. The jammed region is also reflected in the distribution of $\dot{\gamma}_{square}$, with a large region of vanishing shear rate, i.e. $\dot{\gamma}_{square} \rightarrow 0$. Suspensions we discussed here are consisting of frictionless particles, i.e. the volume fractions within the defined jammed area are still below the jamming volume fraction, which indicates that the invalidation of SBM is more likely related to the vanishing shear rate rather than the “over-compaction” where $\phi > \phi_m$.

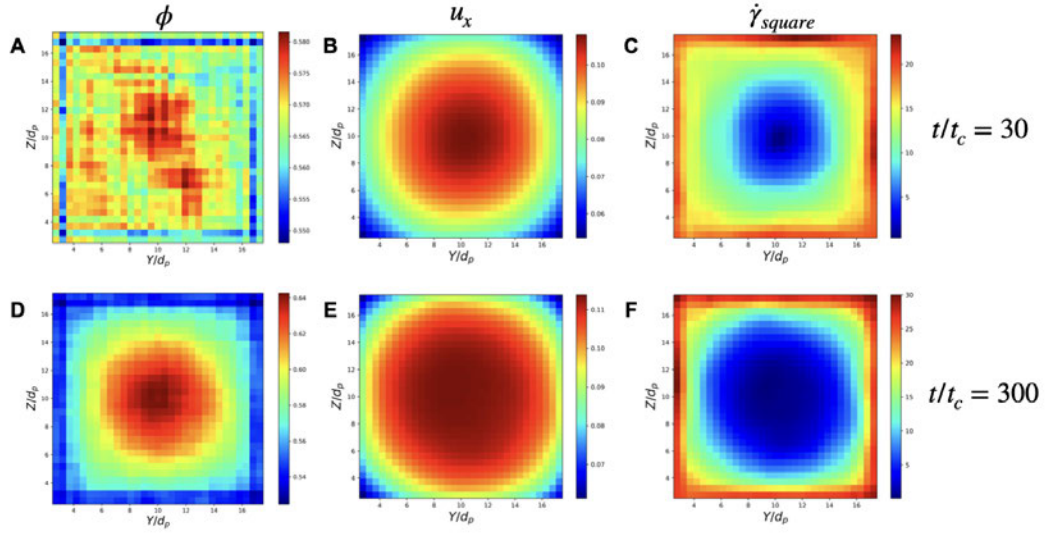


Figure 6.17 The comparison between distributions of (A,D) ϕ , (B,E) u_x and (C,F) $\dot{\gamma}_{square}$ at $t/t_c = 30$ and $t/t_c = 300$.

6.3.3 $\mu(\phi)$ rheology

As discussed in Chapter 5, a critical macroscopic friction coefficient μ_J (where $\mu = \tau/P$) exists for sheared suspensions [11]. However, in the jammed region of pressure-driven suspension flow, the shear stress approaches zero ($\tau \rightarrow 0$) with the vanishing of the shear rate, while migration driven by the particle pressure P^p sustains. This indicates the existence of a region in which the macroscopic friction coefficient μ is less than μ_J . Thus, we can find a region, where $\phi > \phi_m$

and $\mu < \mu_J$, in the channel of the developed suspension consisting of frictional particles. The $\mu(\phi)$ rheology is revisited in this section.

The distribution of ϕ , $\mu = \tau_{square}/P$, V_x and $\dot{\gamma}_{square}$ for $\phi_0 = 0.55, \mu = 0.5$ at $t/t_c = 300$ is shown in Figure 6.18. As expected, a over-jammed area, $\phi > \phi_J$, and a region where macroscopic friction coefficient approaches 0 can be found in Figure 6.18(A,B). The vanishing $\dot{\gamma}_{square}$ is also observed in Figure 6.18(D). Moreover, the symmetry is broken for the spatial distribution of μ and V_x , which is not found in frictionless suspensions(Figure 6.17).

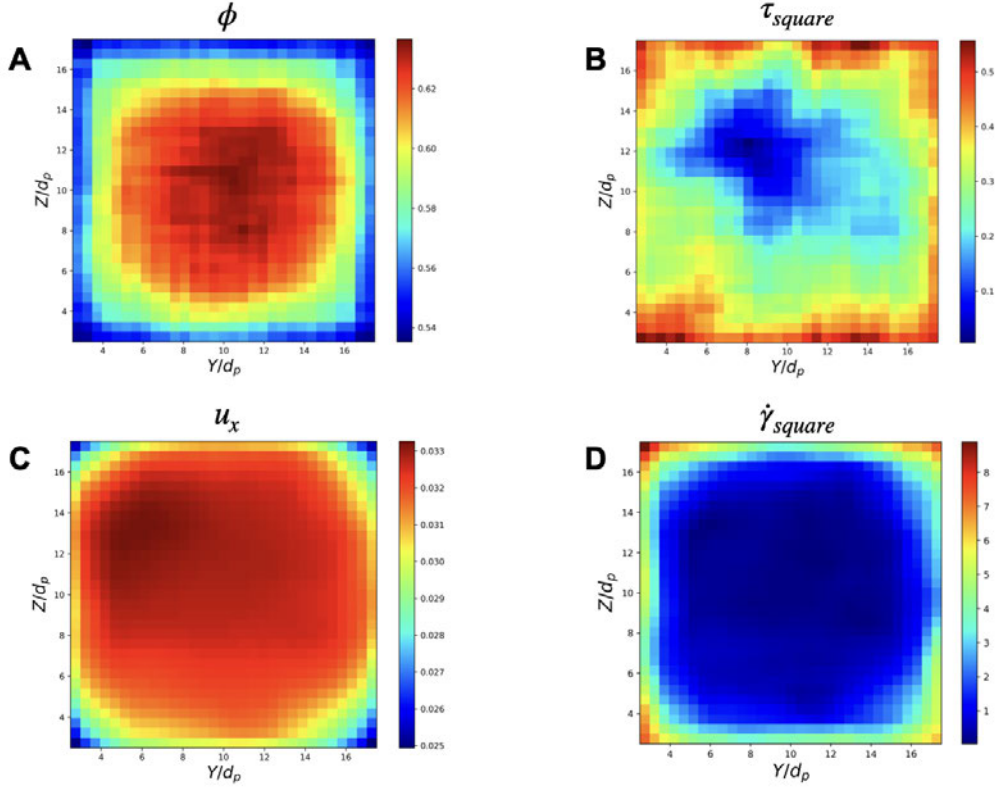


Figure 6.18 Distribution of (A) ϕ , (B) $\mu = \tau_{square}/P$, (C) u_x , (D) $\dot{\gamma}_{square}$ for $\phi_0 = 0.55, \mu = 0.5$ at $t/t_c = 300$.

With the averaged values of Z , ϕ , μ and $\dot{\gamma}_{square}$, we can find the relationship between these quantities. The inset of Figure 6.19(B) is the scatter plot of μ and ϕ for each investigated bin. Averaging over the points with a given ϕ region, e.g. $0.57 < \phi < 0.58$, we can get the averaged ϕ and corresponding μ in Figure 6.19(B). Results shown in Figure 6.19 and 6.20 are taken from $t/t_c > 720$, where the suspensions are estimated to be the developed state. A significant difference can be observed between simple sheared suspensions and pressure-driven suspension in $Z(\phi)$ and $\mu(\phi)$. The contact number is much smaller than the sheared suspension with $Z < 4$ even in the region $\phi \rightarrow \phi_{RCP}$. $Z(\phi)$ is dependent

on ϕ_0 and μ_p . μ constantly decreases to 0 with an increasing ϕ , regardless a critical μ_J in sheared suspension. The ϕ_0 and μ_p dependence is also observed in $\dot{\gamma} - \phi$ relationship, with two clear curves distinguished by μ_p (Figure 6.20). The shear rate vanishes with ϕ approaching ϕ_{RCP} .

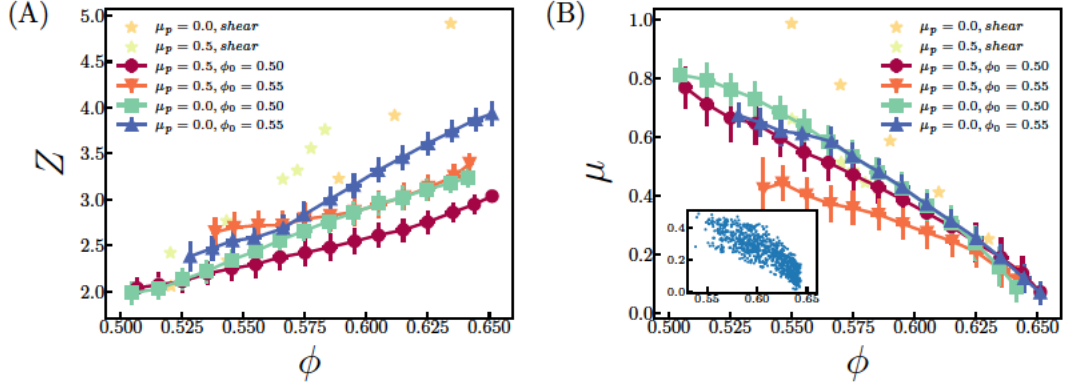


Figure 6.19 (A) Contact number Z as a function of ϕ . (B) μ as a function of ϕ . Inset is the scatter plot of $\mu - \phi$. Scatter diamonds are results of simple sheared suspension taken from Chapter 5.

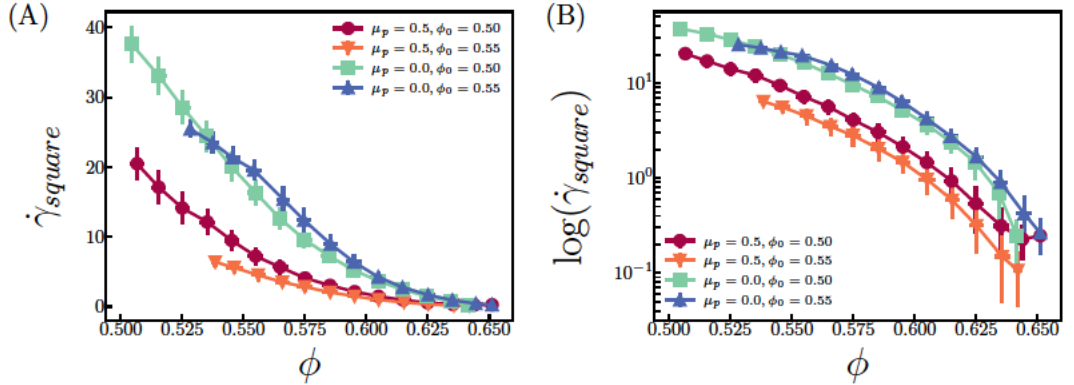


Figure 6.20 Shear rate $\dot{\gamma}_{square}$ as a function of volume fraction ϕ in (A) linear and (B) semilogarithmic scale.

6.4 Discussion & Conclusion

6.4.1 Migration process

Our LBDEM simulation of pressure-driven suspension flow successfully reproduces the shear-induced migration and over-compaction, which is reported in recent experiments for high ϕ_0 [102] but not predicted by conventional theoretical

model[100][11][92][37], near the centre of the channel. The transient dynamics of the migration process, including the shear-induced migration in the sheared region and the over-compaction in the jammed region, are fully captured by our simulation. With the solid and fluid phase information, the suspension balance model is verified at different stages of the migration process. At the beginning of the migration ($t/t_c = 30$), i.e., most areas of the channel are in the sheared regions (Figure 6.17(C)), SBM works well in connecting pressure gradient and migration flux, with different fitting parameters for frictional and frictionless particles. When the suspension is partially developed ($t/t_c = 300$), the jammed region, where $\dot{\gamma} \rightarrow 0$ (Figure 6.17(F)), becomes evident in the channel, SBM fails to capture the migration flux with the pressure gradient. Within the jammed region, particle rearrangements persist and generally evolve to the final developed state.

6.4.2 Non-flowing plug

According to our simulation results and existing experimental and numerical results[92][136][100][123], the SBM based on the homogenous rheology ($\mu(I)$ rheology by Boyer et al. [11]) is useful for conceptualising and predicting the particle distribution in the sheared regions[25] for sheared regions. However, the utility of SBM is limited in capturing the jammed region, also named the non-flowing region where the shear rate approaches 0. Our simulation results suggest the existence of a region in the developed channel, where $\dot{\gamma} \rightarrow 0$, $\phi > \phi_J$ (over-compaction) and $\mu < \mu_J$ (sub-yielding). ϕ_J and μ_J here are critical values at the jamming limit for sheared frictional suspensions. In this region (non-flowing plug), particle rearrangements are dominated by particle fluctuations. According to the frictional model proposed by Lecampion and Garagash [75], the jammed region is constantly excited by perturbations from the nearby flowing region, similar to the liquefaction of granular packing by vibrations or external particle pressure/velocity fluctuations, which is supported by the obvious drop of contact numbers in $\phi > \phi_J$ region. However, the model proposed by Lecampion and Garagash [75] is based on linear extrapolation of the homogeneous $\phi(\mu)$, which is proved to be invalid from our simulation results (Figure 6.19). The ϕ_0 -dependent $\phi(\mu)$ relationship suggests that the conventional homogeneous constitutive model $\phi(\mu)$ is not suitable to be applied to inhomogeneous flow.

The migration mechanism behind the pressure-driven dense suspension flow

contains two parts: particle migration induced by the shear gradient in the sheared region, over-compaction and sub-yielding induced by the fluctuation in the jammed region. However, the bridge between these two regions has yet to be established. A recently proposed tensorial model for the microstructure and stress by Gillissen and Ness [32] in dense suspensions of frictional particles that includes the effect of fluctuations can serve as the further investigation of our simulation results.

Chapter 7

Conclusions and Future Work

7.1 Summary and conclusion

The results of this thesis consists of three parts.

The first part is about a binary model system consisting of frictional and frictionless system. We show that the jamming packing fraction ϕ_J is controlled by the fraction of frictional contacts f , which is solely dependent on the fraction of frictional particles in this model system. The relationship between ϕ_J and f can be captured by a nonlinear interpolation (Equation 4.10), modified from a phenomenological model proposed by Wyart and Cates [135], with different power exponents for different inter-particle friction coefficient μ_{in} . The phenomenological comparison between shear thickening and different μ_{in} points out that a mean-field parameter f is inadequate in predicting the rheology of such binary systems. More microstructural details should be taken into consideration for extending the Wyart-Cates model to predict the rheology of binary systems[41].

The second part concerns the lattice Boltzmann coupling discrete element method simulation of suspensions under simple shear. The comparison between DEM and LBDEM suggested that the drastic simplifications by using DEM were justified as obtained suspension viscosities, stress contributions, normal stress differences, and velocity profiles agree well for dense suspensions. The constitutive model ($\mu - I_v$ rheology) proposed by Boyer et al. [11] can describe the rheology of suspension under simple shear simulated by LBDEM. Moreover, we offered an

alternative way, which tunes the onset stress σ^* instead of varying the shear rate, to capture the shear-thickening behaviour with LBDEM. The simulation results are similar to the widely used rate-controlled critical load model.

The third part focuses on the pressure driven flow of dense suspension in a square channel. We captured the transient dynamics of the migration process, including the shear-induced migration and the over-compaction, in the pressure-driven suspension flow by LBDEM. With simulation results from the solid phase and fluid phase, we prove that the suspension balance model works well in the shear region (Figure 6.15) but fails in the jammed region, where the shear rate disappears. We also found the failure of the $\mu(\phi)$ rheology, a constitutive model for homogeneous suspensions, in the developed state of pressure-driven suspensions. According to our simulation results, we suggest that the model of pressure-driven suspension flow has to capture the homogeneous non-zero shear-rate region and the inhomogeneous vanishing shear-rate region (near/in the plug) at the same time. Despite the boundary effect is evident in our narrow ($H/d_p = 20$) square channel, our simulation results can serve as a solid database for constructing a constitutive model considering microstructure and particle-level fluid field.

7.2 Future work

1. Comparison of DEM with short-range lubrication interaction to LBDEM showed that viscosities are somewhat overestimated for frictional particles and contact numbers are overestimated for both frictional and frictionless particles. A further investigation on the microstructure, including contact numbers and velocity correlations, as suggested by Gallier et al. [31], would be necessary.
2. As discussed in Chapter 6, the dynamics in the jammed region is caused by the propagation of particle fluctuations from the nearby shear region [75]. However, a constitutive model that can capture these two regions simultaneously is not available. The timescale and propagation of the fluctuation are also worth further investigation.
3. Simulations of pressure-driven shear thickening suspension are conducted whereas the thoughtful analysis has not completed. The rearrangements of solid particles surrounding with repulsive force field in the non-flowing region could be

interesting.

4. Working on a further development of the coupling code between DEM and LBM, especially for the parallel efficiency.

Appendix A

Hermite polynomials in the Boltzmann Equation

In mathematics, the Hermite polynomials are a classical orthogonal polynomial sequence. Like the other classical orthogonal polynomials, the Hermite polynomials can be defined from several different starting points. Here we introduce the “probabilist’s Hermite polynomials” in 1D:

$$H^{(n)}(x) = (-1)^n \frac{1}{\omega(x)} \frac{d^n}{dx^n} \omega(x) \quad (\text{A.1})$$

the weighted function $\omega(x)$ is:

$$\omega(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2} \quad (\text{A.2})$$

The Hermite polynomials for d spatial dimensions are:

$$\mathbf{H}^{(n)}(\mathbf{x}) = (-1)^n \frac{1}{\omega(\mathbf{x})} \nabla^{(n)} \omega(\mathbf{x}), \quad \omega(\mathbf{x}) = \frac{1}{(2\pi)^{d/2}} e^{-x^2/2} \quad (\text{A.3})$$

Here $\nabla_{\alpha_1 \dots \alpha_n}^{(n)}$ is a short notation for n consecutive spatial derivatives:

$$\nabla_{\alpha_1 \dots \alpha_n}^{(n)} = \frac{\partial}{\partial x_{\alpha_1}} \dots \frac{\partial}{\partial x_{\alpha_n}}$$

The first eleven probabilist's Hermite polynomials are:

$$\begin{aligned}H^{(0)}(x) &= 1 \\H^{(1)}(x) &= x \\H^{(2)}(x) &= x^2 - 1 \\H^{(3)}(x) &= x^3 - 3x \\H^{(4)}(x) &= x^4 - 6x^2 + 3 \\H^{(5)}(x) &= x^5 - 10x^3 + 15x \\H^{(6)}(x) &= x^6 - 15x^4 + 45x^2 - 15 \\H^{(7)}(x) &= x^7 - 21x^5 + 105x^3 - 105x \\H^{(8)}(x) &= x^8 - 28x^6 + 210x^4 - 420x^2 + 105, \\H^{(9)}(x) &= x^9 - 36x^7 + 378x^5 - 1260x^3 + 945x, \\H^{(10)}(x) &= x^{10} - 45x^8 + 630x^6 - 3150x^4 + 4725x^2 - 945.\end{aligned}\tag{A.4}$$

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