The Effect of Flexibility on Interaction of Two Fibers Settling in Moderate Reynolds Numbers

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THE EFFECT OF FLEXIBILITY ON INTERACTION OF TWO FIBERS SETTLING IN MODERATE REYNOLDS NUMBERS

by

Ahmed Alhasan

A thesis submitted to the Graduate College in partial fulfillment of the requirements for the degree of Master of Science Chemical and Paper Engineering Western Michigan University August 2016

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THE EFFECT OF FLEXIBILITY ON INTERACTION OF TWO FIBERS SETTLING IN MODERATE REYNOLDS NUMBERS

Ahmed Alhasan. M.S

Western Michigan University, 2016

The behavior of solid particles in a fluid has become an important topic. The need to improve our understanding of the mechanisms of fluid-particle interaction is the motivation for the present work. The characteristics of fibers suspensions depend on the many variables such as flexibility, Reynolds numbers, density and aspect ratio. The aim of this work is to probe effects of these variables on sedimentation behavior by using a fiber-level simulation technique. In this techniques, a D3Q15 model in a lattice Boltzmann equation with a Bhatnagar-Gross-Krook (BGK) approximation is used to simulate motion of fluids, where Navier-Stokes equations are solved equivalently. Meanwhile, a lattice spring model is utilized to mimic the deformation of flexible fibers. The interaction between fluid and solid fiber is handled by an immersed boundary method. Dynamic motion of a single flexible fiber and two flexible fibers settling in an infinite long fluid column at low and moderate Reynolds numbers are numerically simulated in a three dimensional space. The fiber flexibility and density are varied at different levels and their effects on sedimentation are studied. In the simulations, cuboid and cylindrical fibers at different aspect ratios are considered. It is demonstrated that the fiber flexibility has an important impact on fiber position, settling velocities, and fluid structures, where the drafting, kissing, and tumbling (DKT) mechanisms play important roles. The simulation results provide useful information, at a microscopic level, which may not be easily measured in a lab environment.
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Ahmed Alhasan
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CHAPTER I

INTRODUCTION

The systems of fluid and suspended solid particles have a wide range of applications in chemical engineering such as pharmaceutical, petroleum, food process, paper industries, and bio-engineering. There are many solid-liquid operations such as fluidized beds in reactors, screening, filtration and sedimentation.

Sedimentation is an important process employed in many industrial processes to separate suspended particles with different sizes from fluids (Ayeni, 2006). For example, in water treatment, sedimentation is commonly used to remove precipitation formed in the processes of water softening (Rong, 2007). In the paper industry, since fines have huge surface areas, receive larger drag forces, and settle slowly by gravity, the sedimentation process can be utilized to separate fines from long fibers. The sedimentation is also used as a primary stage in modern waste water treatment plant, reducing the content of suspended solids as well as the pollutant embedded in the suspended solids. Due to importance to industries, many experimental, theoretical and computational studies are conducted in understanding of the dynamic motion of solid particles in fluid, either coagulation or dispersion, which may help engineers to design a fluid-solid particle handling system with a higher operation efficiency (Ayen, 2006).

In 1987, Fortes et. al. observed experimentally that when two particles sediment vertically in a channel filled with a Newtonian fluid, the trailing particle may accelerate and approach the leading particle, called drafting, due to the suction effect of the low
pressure of the wakes behind the leading particle. When the trailing particle attaches the leading particle, the suction effect is reduced and the two particles becomes unstable, and they exchange their positions. The trailing particle may pass the leading particle position and become the leading particle, called tumbling. This drafting, kissing and tumbling (DKT) phenomena, closely associated with inertial effects, may repeatedly take place during settling process.

Late, Feng al. et [2007] used finite element method (FEM) to simulate the motion of particles settling in a vertical channel and numerically confirmed the DKT phenomenon. Further, many others (Wang al. et, 2014) used different methods to simulate the particle motion and revealed that particle density, initial vertical distance, diameter ratio have a profound influence on the DTK behavior.

Recently using lattice Boltzmann simulations, Wang et. al [2014] reported that when the diameter ratio of two circular particles is smaller than 1.21, DKT phenomena is repeated many times and when the diameter ratio is larger than 1.22, DKT occurs only once.

A recent literature search reveals that most of current works concentrate on either rigid particle in a finite Reynolds number in fluids or flexible particles at Zero-Reynolds number flows. Limited works were reported on flexible or deformable particles at moderate Reynolds numbers where inertia cannot be ignored although sedimentation of fibers (Liu et. al, 2011) at Stokes fluid were extensively studied. The flexible fiber suspension has much more complex dynamic behavior than a rigid particle system because of the complexity of the fiber motion in suspensions. For example, the flexible fiber tends
to deform when subjected to hydrodynamic or colloidal forces and takes on a variety of equilibrium shapes. The dynamics of flexible fiber suspensions depend heavily on the shape and flexibility of the individual fibers as well as the interactions between fibers (Switzer, 2002).

To our best knowledge, only work for flexible fibers at moderate Reynolds numbers is that Wu et al. [2014] employed a flexible particle method, based on lattice Boltzmann simulations, to simulate single and multi-flexible fibers and they learned that a flexible fiber has a larger settling velocity than a stiff fiber and multi flexible fibers may have significantly larger settling velocity than the corresponding isolated single fiber. However, they did not explore the DKT behavior of two flexible fibers.

Therefore, the present work will employ a lattice-spring lattice-Boltzmann method to mimic DKT phenomena of two flexible fibers settling down in an infinite long rectangular fluid channel at a moderate Reynolds number range. In the simulations, flexibility, fiber density, shape and aspect ratio are varied at different levels and their effects on the DKT behavior and fluid structures are investigated.

The rest of this chapter will focus on some literatures review. The next chapter shows the objective of this work. In chapter 3, lattice-spring lattice-Boltzmann method will be briefly introduced. The governing equations used in the simulations is presented in chapter 4. The simulation results of single and two flexible fibers are reported in chapter 5 and some conclusions are made in the last chapter.
1.1 Literature Review

There are many experimental, theoretical and computational studies that shed light on particle flows. A number of methods have been employed and developed to model liquid-solid systems and capture the behavior of settling suspensions, especially in the dilute limit where there are only a small number of particles (Ghosh, Stockie, 2015).

Back in 1851, G.G.Stokes worked on describing fluid properties. He derived an analytical solution to describe the motion of a sphere particle settling within a viscous unbounded fluid. Stoke’s law, “a mathematical description of the force required to move a sphere through a quiescent”, was the basis of solving other more practical sedimentation problems (Shearer, 2010).

The arbitrary Lagrangian Eulerian scheme is the most traditional model which is based on finite element method. In this method, there are no-slip boundary conditions on the surface of each particle. It has been used for the fluid and solid phases respectively but it was employed for very few particles because the meshes’ motions are along with solid particles, so re-meshes are needed. The re-meshing process certainly leads to an increase in computational load and limits the system with a small number of particles.

Later, a Lagrange-multiplier method was presented by Glowinski et al. (1999) with others; Patankar et al. (2000); Wan. & Turek. (2006); Glowinski et al. (2001). Their method reported the motion of large numbers of rigid particles in a Newtonian fluid and used fixed structured grid for finite element formulation to avoid the re-mesh process. However, their work is somehow limited to rigid solid particles.
Further, in 1977 Peskin developed an immersed boundary method (IBM) to be an effective method for solving complex fluid-structure interaction problems that include dynamic moving structures. This numerical method has been used to simulate sedimentation of multiple rigid fibers suspended in a viscous incompressible fluid. Later, Fogelson & Peskin (1988) proposed an immersed boundary method (IBM) for particulate flows.

Fortes et al. observed experimentally that when two particles sediment in a channel filled with a Newtonian fluid, they will touch each other once or more. They will interact undergoing repeated drafting, kissing, and tumbling (DKT), which is called the DKT process. Other researchers used finite element method (FEM) to simulate the motion of particle sedimentation in a vertical channel to get the DKT phenomenon such as the works of Feng and others. They also analyzed the fluid-particle, particle-wall and particle-particle interactions. Ritz and Caltagirone (1999) used finite volume method to simulate the motion of fluid particles and predicted the DKT phenomenon (Wanga, Guo, Mi, 2014).

Mukundakrishnan et. al (2008) and others numerically showed the effect of diameter ratio and density on particle motion and flow behaviors. Shao et. al (2005) and others used the DLM/Fictitious Domain method to investigate the motion of two circular particles with different sizes. They studied the effect of diameter ratio on the interaction of two sedimentation circular particles and they got the DKT process repeatedly with small diameter ratio (below 1:111). They also found that by decreasing the diameter ratio, the DKT will increase, and by increasing the diameter ratio to some extent the two particles will be tumbling and start to separate. In addition, they discovered that the small particles
have more strong influence on the motion of the fluid particles’ interaction than the large particles (Wang et al., 2014).
CHAPTER II

THESIS OBJECTIVES

In recent years, many scientists have theoretically and experimentally studied the sedimentation of solid particles. Most of the works were limited to either rigid fibers or low Reynolds number flows where inertia of fluid and particles was ignored. The focus of this work would be on particle-liquid systems where the density ratio is substantially greater than one.

The general context of this present work deals with two flexible particles-flow problems settling in moderate Reynolds numbers. Comparing and analyzing the effect of the flexibility EI, Reynolds numbers Re, fiber density $\rho$ and aspect ratio, $\kappa = l/d$ where $l$ is the fiber length and $d$ is fiber width, are proposed for single and two particles sedimenting in a three-dimensional channel with infinite length.

The sedimentation process of particles is influenced by many vital variables factors such as particle density, shape and surface properties. In most cases, the particle size, Reynolds number, viscosity, and fiber flexibility are the most significantly influenced factors of sedimentation applications.
CHAPTER III

THEORY AND METHODOLOGY

3.1 Lattice Boltzmann

Navier-Stokes equations describe the motion of viscous fluid substances. These equations could be solved by many traditional computational fluid dynamics (CFD) (Oztekin, 2014). One approach that has proven to be especially effective for solving the complex fluid-structure interaction of Navier-Stokes equations is the lattice Boltzmann method (LBM). By developing the lattice Boltzmann method to predict numerical system and provides interfacial dynamics and complex boundaries, it could successfully simulate fluid flow (Chen and Doolen, 1998). In the solid particle system, the particles are governed by Newton’s equations of motion whereas the Navier-Stokes equations govern the fluid flow. The Lattice Boltzmann method is used to solve these extremely complex systems to get the hydrodynamic forces between the particle and fluid (Chen and Doolen, 1998).

Ladd is the first person who applied lattice Boltzmann equation to particle–fluid suspensions (Wanga, Guo, Mi, 2014). Ladd suggested a modified bounce-back rule to account for the boundary velocity of a moving particle. In the fluid flow, the solid particles are represented by a nodal network system. The momentum exchanges are calculated by the Newtonian dynamics which can be used to calculate the hydrodynamic force and torque on the particle. This method is very popular now because it is very successful in simulating fluid flows (Ladd, 1993).
Many features distinguish the kinetic of the lattice Boltzmann equation from other numerical methods. For example, the streaming process of the lattice Boltzmann equation is linear which contrasts with the other nonlinear numerical methods which use a macroscopic representation. Navier-Stokes (NS) equations can be derived from the lattice Boltzmann equation (LBM) when Mach number is small. If we use direct numerical methods to solve Navier-Stokes NS equations then we have to use the Poisson equation with velocity strains acting as sources to get the pressure and that often produces numerical difficulties requiring special treatment, such as iteration or relaxation (Chen and Doolen, 1998).

The lattice Boltzmann equation (LBE) is a minimal form of the Boltzmann kinetic equation. Solving the Boltzmann kinetic equation directly is not easy because it usually required to solve the equations of continuum fluid mechanics. However, the simulation of the dynamic behavior of fluid flows is meant to solve the equation. Macroscopic fluid dynamics emerge from the underlying dynamics of a fictitious ensemble of particles, whose motion and interactions are confined to a regular space time lattice (Chen and Doolen, 1998).

The probability of finding particles within a certain range of velocities at a certain range of locations replaces tagging each particle as in a molecular dynamics simulation. The lattice Boltzmann transportation can be governed by a distribution function which represents particles at location \( r \) and time \( t \).
3.2 $D_3Q_{15}$ Lattice Model

It is necessary to apply an appropriate collision term satisfying the conservation law of the flow. A 3D incompressible fluid flow with density $\rho$ and kinematic viscosity $\mu$ is simulated in a computational domain that is divided into a regular lattice. The Bhatnagar-Gross-Krook (BGK) model and the $D_3Q_{15}$ model are used for the collision term and the velocity model, respectively.

Figure 1: $D_3Q_{15}$ lattice model
In this discretization scheme, the fluid at each node moves to its neighboring nodes at different velocities or rests with zero velocity.

In a three dimensional lattice, each node has 14 direct neighbor’s particles. If we propose that we consider only the relation from a node to its nearest neighbors in a single time step, that is means, each node has 14 immediate neighbors which gives 15 allowed’ velocities (including a ‘rest velocity’ for stationary molecules). These velocities are expressed as \( i \) \((i = 0…n)\) where \(n\) is the number of allowed velocities. On a lattice, the continuous velocity distribution is divided into components. These components are considering as the fraction of the total mass of fluid at a node that is moving with each of the allowed velocities. We use only 15 allowed velocities as shown in figure (1). Model has one rest direction (0), six orthogonal directions (1...6) and eight diagonal directions (7...14). In other words, the so called D\(_3\)Q\(_{15}\) lattice model (three dimensional, fifteen velocities) is used for the velocity model.

3.3 DKT Phenomenon

The drafting, kissing, and tumbling (DKT) phenomenon occurs between particles settling in a fluid. This phenomenon passes through three stages. First, the upper particle is accelerated by the low-pressure wake of the lower particle. This is a drafting stage. Then, the upper particle contacts and kisses the lower particle aligned with the stream, called the kissing stage. While in the tumbling stage, the kissing particles tumble into more stable cross stream pairs of doublets which can aggregate into larger relative stable horizontal arrays (Wang et al, 2014).
CHAPTER IV

GOVERNING EQUATIONS

In simulations, we use a lattice Boltzmann method to equivalently solve Navier-Stokes equation when the March number is smaller than 0.3 and use a lattice-spring model to mimic deformation of flexible fibers. It is pointed out that the sedimentation behavior of a fiber is mainly determined by hydrodynamic force, fiber elasticity, and gravity. The fiber motion and its deformation can be approximated by a beam motion equation while the fluid follows Navier-Stokes equations. These equations can be non-dimensionalized if the length, velocity, time and force are re-scaled by the fiber length $L$, reference velocity $V_0$, time $L/V_0$, and $\mu V_0 L$, respectively, where $\mu$ is the viscosity. The non-dimensional Navier-Stokes equations for fluids can be written by

$$\nabla . u = 0 \quad (1)$$

$$R_{sd} \left( \frac{\partial u}{\partial t} + u.\nabla u \right) = -\nabla p + \nabla^2 u \quad (2)$$

where $R_{sd} = V_0 L/\nu$ is the particle Reynolds number, $p$ is the pressure, and the non-dimensional beam equation can be written by

$$EI * \frac{\partial^4 w}{\partial t^4} + \frac{\rho_s}{\rho_f} \frac{\partial w^2}{\partial t^2} = \frac{L^2 F_f}{DBR_{sd}} + \left( \frac{\rho_s}{\rho_f} - 1 \right) Fr^{-1} \quad (3)$$

where $l$ is the coordinate variable along the fiber length direction; $w$ is the displacement, due to bending, perpendicular to the fiber length and width directions; $F_f$ is the non-
dimensional hydrodynamic force distributed on the fiber per unit length; $D$ is the thickness of the fiber; $B$ is its width; The rigidity for fibers can be normalized by

$$EI = \frac{EI_l}{\rho_f \cdot V_0^2 \cdot H \cdot L} \quad (4)$$

$H$ is the volume of the fiber; $EI_l$ is the rigidity; The Froude Number is a dimensionless parameter defined as the ratio of the fluid inertia to the gravity.

$$Fr = \frac{V_0^2}{g \cdot l} \quad (5)$$

where $g$ is the gravity acceleration; $l$ is fiber length. It is seen that the first term of the left side of equation 3 is related to fiber rigidity and the second term is a fiber inertial term while the first term of the right side is associated with the hydrodynamic force and the second term comes from the gravity or buoyancy force. The fiber deformation and motion can be determined by a normalized rigidity $EI$, the fiber and fluid inertia, hydrodynamic force, and the gravity force. The gravity force drives fibers to settle down vertically and the fibers may be deformed due to their elasticity while the fiber rigidity and fluid forces may resist the deformation. The dynamics of the flexible fibers are characterized by dimensionless elasto-gravitation number $\beta$ that is defined by a ratio of the rigidity $EI$ to the buoyancy force as

$$\beta = \frac{EI \cdot Fr}{\rho_p - 1} \quad (6)$$

Here: $\rho_p$ is particle density; $\rho_f$ is fluid density. A larger elasto-gravitation number may result in a smaller deformation and vice versa. This number is useful for analysis of effects of the rigidity and gravity on the deformation.
4.1. Lattice Boltzmann Equations

The Navier-Stokes equations describe the motion of viscous fluid substances. These equations could be solved by many computational fluid dynamics (CFD) methods. The lattice Boltzmann method (LBM) has been proven to be especially effective for solving the fluid flows interacting with complex solid boundaries. Fluid particles are located on lattice nodes. The fluid particles move to their nearest neighbors along the links with unit spacing in each unit time step. Each node has distribution functions $f_\sigma$ and discrete micro-velocity $e_\sigma$, where $\sigma$ depends on the chosen lattice model. The lattice Boltzmann equation with Bhatanaga-Gross-Krook BGK single relaxation time is given by (Guo, Zheng & Shi, 2002)

$$f_\sigma (\vec{r} + \vec{e}_\sigma , t + \delta t) = f_\sigma (\vec{r},t) - \frac{1}{\tau} \left( f_\sigma (\vec{r},t) - f_{eq}^\sigma (\vec{r},t) \right) + \delta t \cdot \vec{F}_\sigma (\vec{r},t)$$

(7)

In the equation above $f (\vec{r},t)$ represent the fluid particle distribution function for particles with velocity $\vec{e}_\sigma$ at position $r$ and time $t$. $f_{eq}^\sigma (\vec{r},t)$ is the equilibrium distribution function.

Subscript $\sigma$, indicates the type of particle and $\tau$ indicates the single relaxation time which controls the rate of approach to equilibrium. $\vec{F}_\sigma (\vec{r},t)$ is the body force.

The left hand side of equation (7) represents the discrete velocity of the Boltzmann streaming operator while the right hand side corresponds to the particle collisions through a relaxation to a local equilibrium (Guo, Zheng & Shi, 2002). $f_{eq}^\sigma (\vec{r},t)$ is obtained by
expanding the Maxwell Boltzmann distribution function in Taylor series of $u$ up to the second order and it is defined as:

$$f_{\sigma}^{eq} (\vec{r},t) = \omega_{\sigma} \rho_f \left[ 1 + 3(\vec{e}_{\sigma} \cdot \vec{u}) + \frac{9}{2} (\vec{e}_{\sigma} \cdot \vec{u})^2 - \frac{3}{2} (\vec{u} \cdot \vec{u}) \right]$$  \hspace{1cm} (8)

Where $\omega_{\sigma}$ is the weighting factor which is given according to (Qi, 2006) by

$$\omega_{\sigma} = \begin{cases} 
\frac{2}{9}, & \sigma = 0 \\
\frac{1}{9}, & \sigma = 1 \\
\frac{1}{72}, & \sigma = 2 
\end{cases}$$

In this simulation, the D$_3$Q$_{15}$ lattice model is applied and the discrete velocity is given by

$$\vec{e}_{\sigma} = \begin{cases} 
(0,0,0) & \sigma = 0 \\
(\pm1,0,0) & \sigma = 1 \\
(\pm1,\pm1,\pm1) & \sigma = 2 
\end{cases}$$

$$F_{\sigma} = (1 - \frac{1}{2\tau})w_{\sigma} \left( \frac{e_{\sigma} - u}{c_s^2} + \frac{e_{\sigma} \cdot u}{c_s^3} \right) \vec{e}_{\sigma} \right) \cdot \vec{F}$$ \hspace{1cm} (9)

$F$ is the body force, $F_{\sigma}$ is its component in the $\sigma$ direction. $c_s^2 = 1/3$ where $c_s$ is the sound speed; the fluid density $\rho_f$ and momentum density $\rho_f \vec{u}$ are given by

$$\rho = \sum_i f_i$$ \hspace{1cm} (10)
\[ \rho \mathbf{u} = \sum_i f_i \mathbf{e}_i + \frac{1}{2} \delta t \mathbf{F} \]  

The kinematic viscosity \( \nu \) is related to the relaxation time \( \tau \) and is given by (Wu & Qi, 2014):

\[ \nu = \frac{1}{3} (\tau - \frac{1}{2}) \delta t \]  

When the cases of Reynolds number \( (Re=0) \) are simulated, the terms with the second order of velocity in the fluid particle distribution function given by Eq. (2) are not included. A moving boundary condition by Ladd is used to match the fluid velocity with the solid boundary velocity at the fluid-solid interface (Dewei, Liu, Shyy, & Aono, 2010):

\[ f_{\sigma'}(\mathbf{x}, t+1) = f_\sigma(\mathbf{x}, t) - 6 \omega_\sigma \rho \mathbf{e}_\sigma \cdot \mathbf{U}_b \]  

where \( \sigma' \) represents the reflecting direction and \( \sigma \) denotes the incident direction of fluid particle at a node adjacent to the solid-surface with the boundary velocity \( \mathbf{U}_b \)

\[ \mathbf{U}_b = \mathbf{U}_C + \mathbf{\Omega} \times \mathbf{x}_b \]  

where \( \mathbf{U}_C \) is the velocity of the mass center of the corresponding solid particle; \( \mathbf{\Omega} \) is solid particle angular velocity; \( \mathbf{x}_b = \mathbf{x} + \frac{1}{2} \mathbf{e}_\sigma - \mathbf{R}_i \); \( \mathbf{x} \) is the position of the node; \( \mathbf{R}_i \) is the mass center of the solid particle. The hydrodynamic force exerted on the solid particle at the boundary node is computed by (Dewei, Liu, Shyy, & Aono, 2010):
\[ \bar{F}(\bar{x} + \frac{1}{2}\bar{e}_\sigma) = 2\bar{e}_\sigma (f_\sigma (\bar{x}, t_s) - 3\omega_\sigma \rho_f \bar{U}_b \cdot \bar{e}_\sigma) \]  

(15)

4.2. Flexible Fiber Model

The Lattice Boltzmann Flexible fiber model (LBFPM) has been reported by (Qi, 2006). In this model, the fiber is represented by a chain of rigid cylindrical parts. These segments contact each other through ball and socket joints. The long fibers may be bent and twisted through relative rotation between the segments. The length of each cylindrical segment is \( l = L/N = 2d \); where \( N \) is the total number of cylindrical segments in a fiber; \( L \) is the fiber length. One end of a cylindrical segment always contacts the end of its nearby segment that the segment can rotate in three dimensional space around the joints as shown in Figure (2).

![Figure 2](image)

Figure 2: The beam segments are connected through ball and socket joints. (The figure from Qi, 2006)
During fiber motion, the following condition has to be applied:

\[ R_{i+1} - C_{i+1} = R_i + C_i \quad i = 1, N-1 \]  

(16)

where \( R_i \) is the mass center of the \( i \)th fiber segment and \( C_i \) is the vector from its mass center to the joint \( i \), where \( i \) runs from 1 to \( N-1 \) and the cylindrical segments are labeled by index \( i \) in increasing order (Qi, 2006).

4.3. Lattice-Spring Model

Based on Hooke’s Law, Buxton et al. (2005), provided the lattice spring model to represent the interparticle force between the elastic structure. In the method, the fiber is discretized as individual particles with a mass of \( m \) for each particle, which are connected by bonding harmonic elastic springs and angular elastic springs to ensure that three body force is added into model so that it can handle the bending deformation (Wu et al. (2014)). Thus, the spring energy \( U_s \) acted on the \( i \)th node is given by

\[ U_i^s = \frac{1}{2} k_s \sum (r_{ij} - r_{0ij})^2 \]  

(17)

Where \( k_s \) is the spring coefficient, \( r_{0ij} \) is the equilibrium length of the spring between two neighboring particles \( i \) and \( j \); \( j \) is the nearest neighboring solid particle of the \( i \)th solid particle. \( r_{ij} = r_i - r_j \). The angular energy \( U_a \) is given by

\[ U_i^a = \frac{1}{2} k_a \sum_{jk} \sum_{k \neq j} (\theta_{ijk} - \theta_{0ijk})^2 \]  

(18)
Where $k_a$ is the angular bonding coefficient; $j, k$ are the nearest neighboring solid particles of $i$ th solid particle; $\theta_{ijk}$ is the angle between the bonding vectors $r_{ij}$ and the bonding vector $r_{ik}$; $\theta_{0ijk}$ is the corresponding equilibrium angle.

Figure 3: The solid particles are located in a cubic lattice and the particle lattices are linked by springs and angular bonds.

4.4. Kinematics of Moving Particle

The elastic force $F_i^e$ on the $i$ th solid particle can be computed from the gradient of the total energy:

$$F_i^e = -\nabla(U_i^s - U_i^a)$$

(19)
The elastic modulus of the solid body can be related to the spring and angular coefficients. The relationship between elastic modulus $E$ and shear modulus depends on lattice structure. For a cubic lattice structure without diagonal bonds (Wu et al, 2014), we have

$$E = \frac{k_s}{r_0}$$

(20)

where $r_0$ is the distance between particles $i$ and $j$ if the solid material is isotropic.

In order to force the fluid velocity equal to the solid boundary velocity at the fluid-solid interface, a direct forcing-force $F$ should be added to the un-forced fluid velocity $u^* (r^b, t)$ to make the fluid velocity equal to the solid boundary velocity at the fluid-solid interface. According to Newton's second law, the momentum summation is equal to the solid boundary velocity $u^b (r_b, t)$. According to the Newtonian second law. This is

$$\rho_f u(r^b, t) = \rho_f u^* (r^b, t) + \delta t F = \rho_f U^b (r^b, t)$$

(21)

$u(r^b, t)$ is the forced fluid velocity at $r^b$ (the solid boundary position), $u^* (r^b, t)$. The un-forced velocity is calculated by

$$\rho_f u^* = \sum_{\sigma} f_{\sigma} e_{\sigma}$$

(22)

Therefore, the direct forcing force on fluid can be calculated by
\[ F(r^b, t) = \frac{\rho_f (U^b_r(r^b, t) - u^*(r^b, t))}{\delta t} \]  

(23)

The force acting on the solid boundary node by fluid is \(-F(r^b, t)\). The un-forced fluid velocity \(u^*\) at the position of the solid boundary node \(r^b\) is presented by

\[ u^*(r^b, t) = \int_{\Pi} u^*(r^l, t) D(r^l - r^b) dr^l \]  

(24)

where \(r^l\) is a variable. Since the fluid node position may not be coincided with the solid particle position, the fluid velocity on the boundary solid node can be approximately extrapolated from the fluid velocity of the surrounding solid boundary node by using a discrete Dirac Delta function (Wu, 2014)

\[
D(r) = \begin{cases} 
\frac{1}{64h^3} \left( 1 + \cos \frac{\pi x}{2h} \right) \left( 1 + \cos \frac{\pi y}{2h} \right) \left( 1 + \cos \frac{\pi z}{2h} \right) & \text{if } |r| \leq 2h \\
0 & \text{otherwise}
\end{cases}
\]

where the \(h\) is the one lattice unit length. The fluid nodes are within a spherical volume \(\Pi\) of a radius of \(2h\), centered at a given solid node \(r^b\). It is noted that the fluid forcing force needs to be calculated by using equation 23. Its physical meaning is that based on momentum conservation, the forcing force is added to unforced fluid particle and ensure its velocity equal to the solid particle velocity. Only after the forcing force is obtained from equation 23, fluid velocity can be calculated by using equation 22. The forcing term components \(\delta t F_\perp\) are added into fluid following equation 7. Then, the discrete Dirac delta function is utilized again to distribute the reaction force to the surrounding fluid nodes.
\[
F(r^i, t) = \int_{\Gamma} F(r^b, t) D(r^i - r^b) dr^b
\]  
(25)

where \( F(r^i, t) \) is the distributed force and \( \Gamma \) is a spherical volume of a radius of \( 2h \), located at \( r^j \).

In addition, to avoid two fiber overlap during simulations, the repulsive portion of the Lennard-Jones potential is employed between the solid particles in different fibers.

\[
U_{IJ} = \epsilon \left( \frac{\sum}{r_{ij}} \right)^{12}
\]  
(26)

\( \Sigma \) is a force interaction diameter and \( \epsilon \) is the parameter of the intensity of the repulsion.

The total force on a discretized solid particle \( i \) is

\[
F_{ij}^T = -F_i (r^b) + F_i^e + F_{ii,J}
\]  
(27)

where \( F_{ii,J} \) is the force on the \( i \)th particle due to the repulsive Lennard-Jones potential. It is critical to select correct values of the parameters \( \Sigma \) and \( \epsilon \) to assure the approximation of momentum conservation during collision. Next, the leap frog algorithm is taken to update the position and velocity of each solid particle at each time step by using Newtonian mechanism. The details about the leap frog algorithm is referred to Chapter 3 of the book by Allen and Tildesley [1987].
5.1 Simulation Setup

Our main motivation for this study is to investigate and analyze sedimentation of flexible fibers. In this chapter, main results of flexible fiber suspension have been presented.

To display and describe the overall effects (within the established parameters) of the motion of flexible fibers in fluid, simulations have been conducted. These calculations have been done in many simulation cases. A code program has been used to simulate the interaction between flexible fibers and how they settle in a fluid.

An infinite long rectangular simulation box of \((N_x, N_y, N_z) = (60, 160, 650)\) is used. Fibers with zero velocity are initial located in the center of the simulation box, then released, and settle down in the vertical or z-direction by gravity. Whenever the fiber moves down one grid distance, the fluid layer at the top grids is removed and another fluid layer is added in the bottom grids. Meanwhile, to ensure the free surface for the top fluid flow, the fluid velocity gradient in the vertical direction is satisfied by \(\frac{\partial V_z}{\partial Z} = 0\). The bottom fluid flow velocity is set as zero. Two walls are set at the ends of the simulation box in the x-direction and periodic boundary conditions are imposed in the y-direction.
In all cases, the same fluid parameters have been used: density \( \rho_f \) and viscosity \( \mu_f \) are set to 1.0 g/cm\(^3\) and 0.04 g/cm s, respectively. All dimensions are used with lattice units.

In all of the figures of this work, displacement has been normalized by \( L/L_o \); \( L_o \) is particle length, time normalized by \( t/t_o \); \( t \) is the number of steps and \( t_o \) is defined as \( t_o = L/V_o \); where \( V_o \) is the particle velocity at a Stock flow, velocity normalized by \( V/V_o \) unless otherwise specified.

5.2. Validation

To select appropriate grids, three different sizes of the fiber and simulation box are used to test simulation resolution for the same case of \( EI = 0.048, \beta = 0.0036, \rho_r = \rho_s/\rho_f = 1.4, \) and \( Re = 58.94 \). The three rectangular fiber sizes are \( (B,D,L) = (7,7,41), (5,5,29), \) and \( (4,4,23) \) and their corresponding simulation box sizes are \( (N_x,N_y,N_z) = (8.57B, 22.86D, 15.85L) \) as shown in table 1.

Table 1

<table>
<thead>
<tr>
<th>Fiber Size ((B,D,L))</th>
<th>Simulation Box Size ((N_x,N_y,N_z))</th>
<th>Time Step Unit ((s))</th>
<th>Length Unit ((cm))</th>
</tr>
</thead>
<tbody>
<tr>
<td>( (7,7,41) )</td>
<td>( (60,160,650) )</td>
<td>0.000130</td>
<td>0.00806</td>
</tr>
<tr>
<td>( (5,5,29) )</td>
<td>( (43,114,464) )</td>
<td>0.000182</td>
<td>0.0113</td>
</tr>
<tr>
<td>( (4,4,23) )</td>
<td>( (34,91,371) )</td>
<td>0.000229</td>
<td>0.0141</td>
</tr>
</tbody>
</table>
The simulation length unit is 1.75 times and the time step unit is 1.76 times smaller for the finest grid case than for the coarse grid case. The results of the sedimentation velocity of the mass center as a function of time are compared in figure 1 among the finest, middle, and coarse grid cases. No significant difference is observed, indicating the resolution is enough even using coarse grids. However, to guarantee
accuracy, the finest grids of the fiber size of \((B,D,L) = (7, 7, 41)\) and its corresponding simulation box size are used in this work.

To validate the simulation of two particles, two different sizes of the fibers and simulation box are used to test simulation resolution for the same case of \(EI = 0.029, \beta = 0.0043, \rho_r = \rho_s/\rho_f = 1.2, \) and \(Re = 38.95\). The rectangular fiber sizes set to \((B,D,L) = (7, 7, 41)\) and \((5, 5, 29)\) and their corresponding simulation box sizes are \((N_x,N_y,N_z) = (8.57B, 22.86D, 15.85L)\). Figure (5) shows the results of two cases. The settling velocity shows good agreement for the two simulations.

![Diagram showing settling velocity for single particle as a function of time for the same case at three different resolutions.](image)

Figure 5: The settling velocity for single particle as a function of time for the same case at three different resolutions.
CHAPTER VI

THE RESULTS

The settling or terminal velocity of particles is one of the frequently interested variable in study and analysis. The settling velocity of particles is influenced by the fluid dynamic environment and the attributes of the particle, such as its size, shape, and density. Thus, in all next results, the sedimentation velocity has been plotted as a function of time.

6.1. Sedimentation of Single Particle

6.1.1 Effect of Flexibility

To investigate the effect of flexibility on sedimentation of single particle, various cases with different values of rigidity (EI) have been run (Table 1). A single rectangular particle settles in a 3D rectangular channel. At first \( t = 0 \), both particle and flow are set to be rest and then the particle commences its motion downward under the force of gravity because it heavier than the fluid particles.

Table 2

Effect of Flexibility

<table>
<thead>
<tr>
<th>Case No.</th>
<th>fiber Shape</th>
<th>density</th>
<th>Young’s modulus</th>
<th>Elasto-gravitation numbers</th>
<th>Settling velocity</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Cuboid</td>
<td>1.4</td>
<td>0.05</td>
<td>0.0036</td>
<td>0.0575</td>
</tr>
<tr>
<td>2</td>
<td>Cuboid</td>
<td>1.4</td>
<td>0.1</td>
<td>0.0072</td>
<td>0.056</td>
</tr>
<tr>
<td>3</td>
<td>Cuboid</td>
<td>1.4</td>
<td>1.2</td>
<td>0.086</td>
<td>0.055</td>
</tr>
</tbody>
</table>
The simulations are conducted in the same conditions except that the rigidity is varied at three different levels collected in table 2. In these cases, three levels of the rigidity $EI = 0.048, 0.5$ and $1.17$ are used, respectively. The aspect ratio of the fiber is kept at $L/D = 5.86$ and the density ratio $\rho_r$ of the solid to fluid is fixed at $\rho_r = \rho_s/\rho_f = 1.4$ where $\rho_s$ is sold density and $\rho_f$ is fluid density. The results of the settling velocity of the fiber as a function of time are plotted and compared in figure 7. In the figure, the settling velocity is normalized by the settling velocity $V_{0z}$ in a Stokes flow. The Stokes velocity is obtained
by a simulation where the second order term of the velocity in equation 8 and 9 are set as zero. The time is normalized by $t_0 = L/V_0$.

![Figure 7](image)

**Figure 7:** Comparison of the fiber settling velocity as a function of time among three different levels of rigidity.

The deformation due to flexibility plays important roles in settle velocity. It is shown that fibers deformations increase by increase its flexibility. When a fiber settles, it pushes the fluid in the front area and creates a higher pressure in the front of the fiber and a lower pressure in the back of the fiber. The pressure difference will try to move the fluid from the high pressure area to the low pressure area. However, the fluid in the fiber center is not easy to flow to the back side due to the resistant of the solid body. Only the fluid
around the fiber tip area can flow easily to the back side of the fiber and form a circular back flow so that tip vortices are formed as show in figure 8 for the case of $EI = 0.048$.

Figure 8: The velocity fields and tip vortices around the area of the two ends of the single
Figure 9: Velocity flow of the single particle in the vertical (Y) direction with different rigidity, a) at $t/t_0=0.01$, b) at $t/t_0=5$.

A flexible fiber can be deformed more easily and fitted more conformably with the streamlines than a rigid fiber. Therefore, the settling velocity increases as the fiber flexibility increases as shown in figure 9.
Figure (10) shows the curl index C as a function of time. The curl index is defined by $C = L/L_0 - 1$, where $L_0$ is the end-to-end length of the curved fiber. The results clearly show that case 1, fiber with $EI=0.048$, has largest deformation and is the most flexible fiber while the fiber with $EI = 1.166$ (case 3) has the little deformation and is the most rigid fiber.

Figure 10: Fiber curvature index as a function of time
6.1.2 Effect of Reynolds Number

To study the effect of Reynolds number on sedimentation of single particle, five cases have been runs (Table 3). In all cases, the rigidity is fixed at 0.791 and Reynolds number is changed. The Elasto-gravitation numbers (β) are calculated as shown in table. The aspect ratio of the fiber is always fixed at $\kappa = L/d = 5.857$.

Table 3
Effect of Reynolds Number

<table>
<thead>
<tr>
<th>Case No.</th>
<th>Particle Shape</th>
<th>Reynolds Number</th>
<th>Young’s modulus</th>
<th>Rigidity</th>
<th>Elasto-gravitation numbers</th>
<th>Settling velocity</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>cuboid</td>
<td>22</td>
<td>1</td>
<td>0.971</td>
<td>0.24</td>
<td>0.0216</td>
</tr>
<tr>
<td>2</td>
<td>cuboid</td>
<td>56</td>
<td>1</td>
<td>0.971</td>
<td>0.072</td>
<td>0.055</td>
</tr>
<tr>
<td>3</td>
<td>cuboid</td>
<td>74</td>
<td>1</td>
<td>0.971</td>
<td>0.048</td>
<td>0.073</td>
</tr>
<tr>
<td>4</td>
<td>cuboid</td>
<td>90</td>
<td>1</td>
<td>0.971</td>
<td>0.036</td>
<td>0.088</td>
</tr>
<tr>
<td>5</td>
<td>cuboid</td>
<td>104</td>
<td>1</td>
<td>0.971</td>
<td>0.029</td>
<td>0.102</td>
</tr>
</tbody>
</table>

As we know, the settling velocity increases as the fiber density increases if other conditions are fixed. The sedimentation velocity of a fiber is directly proportional with particle Reynolds number. Thus, particle settling velocity increases with increasing particle Reynolds number as shown in Fig (12). In other hand, the elastic gravitational force is inversely proportional with Reynolds number due to increase particle density which leads to increase gravitation force. Figure (13) shows the vorticity flow of the single particle in the vertical (Y) direction with different Reynolds number.
Figure 11: Comparison of the single fibers settling velocity in the vertical (Z) direction with different Reynold number.
Figure 12: Vorticity flow of the single particle in the vertical (Y) direction with different Reynolds number. (a) at $t/t_0=0.01$ (top); (b) at $t/t_0=5$ (bottom).

The fibers with high Reynolds numbers can be deformed more easily and fitted more conformably with the streamlines than lower Reynolds number fibers. Therefore, the settling velocity increases as the fiber Reynolds number increases as shown in figure 13.
Figure (13) shows the curl index C as a function of time among different levels of Reynolds number. The results show that the fibers with higher Reynolds number have larger deformation. Therefore, in general, the deformation of the fibers increases as the fiber Reynolds number increases.

6.1.3 Effect of Fiber Shape

To understand the effect of fibers shape on sedimentation, two different shapes fiber have been prepared for investigation. The sedimentation of rectangular and cylinder fibers has been simulated under the same conditions of fluid properties and simulation. The orthogonal axial lengths for both fibers is 41 lattice units. The cross section area of
the two cases set to 0.000065 cm². The result in figure (14) illustrate that cylinder fiber is settle more rapidly than rectangular fiber because cylinder fibers deform easier than rectangular fibers.

Figure 14: Comparison between settling velocity in the vertical (Z) direction for two different fiber’s shape

6.2. Sedimentation of Two Particles

For comparison, many cases of two rectangular and cylinder particles sedimentation under gravity are simulated under the same conditions by using lattice Boltzmann methods. The two particles rest initially at the middle of a three-dimensional channel. The initial size of the simulation box is 60 x 160 x 900 lattice units. The two particles heavier than the fluid so, they settle by gravity.
6.2.1. Drafting–Kissing– Tumbling (DKT) Phenomena

Two particles of same density and diameter are used in this case. The two particles are named as their order of arrangement. The first particle is called "trailing particle" and the second particle is called "leading particle".

![Figure 15: Tow Particles Simulation Box](image)

The two particles are simulated in a rectangular box. Initially, the two particles are located at the channel centerline. The distance between the two particle is 2D (D is the particle diameter). The two particles have same dimension (7, 7, 41) and same density $\rho = 1.2 \text{ g/cm}^3$. At first (t = 0), both particles and flow are set to be rest and then the two particles commence their motion downward under the gravity force. It is expected that the particles will reproduce the Drafting–Kissing– Tumbling (DKT) phenomena which was first experimentally discovered by Joseph et al. (1987).
In Figure (16), two particles are initially at rest and start to settle under the effects of gravity. The leading particle (particle-2) creates a wake of low pressure, and the trailing particle (particle-1) sliding in the leading particle’s wake. The drag force on the trailing particle will be reduced and make it settles faster than the leading particle. The trailing particle drafts towards the leading particle due to an increase in the settling speed. Then, the two particles will touch each other, called kissing. As mentioned by (Dash, Lee, and Huang, 2014), the kissing of particles is an unstable equilibrium state so the particles will try to breakdown of this state and enter a tumbling stage. The Drafting–Kissing–Tumbling (DKT) phenomena may repeat many times. DKT is a feature of Navier–Stokes flows but it does not exist in Stokes flow. DKT feature is used to test simulations of the finite Reynolds number suspension.
Figure 16: Drafting–Kissing–Tumbling (DKT).
6.2.2. Effects of Flexibility On Two Fiber Sedimentation

The effects of flexibility on sedimentation of two cuboid particles have been studied in the following cases. Four cases with different rigidity and Reynolds number have been run. In all cases, the two particles are located at the channel centerline. The distance between the two particles is 10?? lattice units. Each two particles have same dimension (7, 7, 41) and same density. The aspect ratio of the fiber is always fixed at \( \kappa = \frac{L}{d} = 5.857 \).

In the first two cases, the fibers density set to be 1.2 while the rigidity set as 0.029 and 0.972 respectively. The viscosity (\( \mu = 0.04 \)) and epsilon (\( \varepsilon = 0.08603 \)) are fixed. The young’s modulus for first case (\( E = 0.03, EI=0.029 \)) and for second case (\( E =1.1 \) \( EI=0.972 \)). The Reynolds number of the flexible fiber is \( Re=37.9 \), the Reynolds number of the Rigid fiber is \( Re=32.8 \). The trajectories of vertical velocity \( V_z \) of the flexible and rigid particles are plotted as a function of time step.

Table 4

Effect of Flexibility on Two Fiber Sedimentation

<table>
<thead>
<tr>
<th>Case No.</th>
<th>Particle Shape</th>
<th>Reynolds Number</th>
<th>Density</th>
<th>Young’s modulus</th>
<th>Rigidity</th>
<th>Elasto-gravitation numbers</th>
<th>Settling velocity</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Rectangular</td>
<td>37.9</td>
<td>1.2</td>
<td>0.03</td>
<td>0.029</td>
<td>0.0043</td>
<td>0.038</td>
</tr>
<tr>
<td>2</td>
<td>Rectangular</td>
<td>32.8</td>
<td>1.2</td>
<td>1.1</td>
<td>0.972</td>
<td>0.144</td>
<td>0.032</td>
</tr>
<tr>
<td>3</td>
<td>Rectangular</td>
<td>71.75</td>
<td>1.6</td>
<td>0.1</td>
<td>0.097</td>
<td>0.0048</td>
<td>0.07</td>
</tr>
<tr>
<td>4</td>
<td>Rectangular</td>
<td>71.75</td>
<td>1.6</td>
<td>1.3</td>
<td>1.263</td>
<td>0.062</td>
<td>0.07</td>
</tr>
</tbody>
</table>
Figure 17: The trajectories of vertical velocity $V_z$ (Flexible Particle) at Re=35

Figure 18: The trajectories of vertical velocity $V_z$ (Rigid Particle) at Re=35
In the Figures (17, 18), we can see that settling vertical velocities of the rigid particles (case 2) affected slightly compared to the flexible particles (case 1). In the flexible case, drafting, kissing and tumbling process is repeated more than the rigid case. The mean velocity of first case is 0.038 while for the second case 0.032. We can indicate that the increasing in flexibility will help the two particles to touch and change their position more. The flexibility allows the particle sliding faster. In other words, the sedimentation of flexible particles faster than the rigid particles because of increasing of the wake flow.

When two fibers sediment under gravity, they generate vortices in the tip areas. Figure (19) shows a comparison between sedimentation of two scales of flexible fibers (Case 1) and sedimentation of two rigid fibers (case 2) in different times. Figure (20) shows the velocity field and the vorticity contours in the Z direction in the XY-cross section of the two flexible fibers (Case 1) and two rigid fibers (case 2) in different times.
Figure 19: A comparison between two flexible particles (Case 1) and two rigid particles (case 2) in different times, a) at $t/t_0=0.01$, b) at $t/t_0=4$, c) at $t/t_0=7$. 
Figure 20: The velocity field and the vorticity contours in the Z direction in the XY-cross section of the two flexible particles (Case 1) and two rigid particles (case 2) in different times.
The results of the curl index as functions of time at the two levels of the flexibility are exhibited in Figure (21). It is shown that the deformation of case1 with EI=0.029 is higher than the deformation of case2 with EI=0.972. Thus, deformation increases as the flexibility increases.

Figure 21: Comparison of the curvature index between the two cases of EI = 0.029 and EI = 0.972
The probability of finding a fiber segment having an angle of \( \theta \) with the horizontal direction per unit angle is the angular distribution function \( f(\theta) \). The angular distribution function \( f(\theta) \) which described fibers orientation defined by \( f(\theta) = \frac{\left\langle \sum_i \delta(\theta - \theta_i) \right\rangle}{n} \) where \( \left\langle \cdots \right\rangle \) is the ensemble average; \( n \) is total number of the fiber segment; \( i \) denotes the \( i \)th segment and \( \delta \) is the Dirac function. Figure (22) shows the angular distribution for the flexible and stiff fibers, respectively. The results demonstrate that the stiff fibers have a larger probability to be oriented in horizontal direction than the flexible fibers due to their bending or shape deformation.

![Graph showing angular distribution function for fiber segments between two cases of EI = 0.029 and EI = 0.972.](image)

Figure 22: Comparison of the angular distribution function of fiber segments between the two cases of EI = 0.029 and EI = 0.972.
Figure (22) shows comparison between the angular distribution function for the stiff and flexible fibers. In the cases 3 and 4, the Reynolds number increased by increase particle density to be 1.6. The young's modulus for third case ($E = 0.1$, $EI=0.097$) and for fourth case ($E = 1.3$, $EI=1.263$). Other kinematic parameters are kept the same. (aspect ratio, viscosity, epsilon ... etc.). The trajectories of vertical velocity $V_z$ of the flexible and rigid particles are plotted as function of time steps.

Figure 23: The trajectories of vertical velocity $V_z$ (Flexible Particle) at $Re=71$. 
Figure 24: The trajectories of vertical velocity $V_z$ (Rigid Particle) at Re=71.

The number of Drafting–Kissing–Tumbling (DKT) circle in the third case is more than the fourth case; however, the settling velocity for the both cases is the same (0.07).

The results of the curl index for case 3 and 4 as functions of time at the two levels of the flexibility ($EI=0.097$, $EI=1.263$) are displayed in figure (25). It has been found that the deformation of flexible fibers (case 3) is larger than the deformation of rigid fibers (case 4).
6.2.3. Effects of Reynolds Number On Two Fiber Sedimentation

To assess the effects of the Reynolds number on the sedimentation of two fibers suspensions, additional simulations have been conducted. Four cases have been run with the same conditions except that Reynolds number (Re=1.9, Re=35, Re=71, Re=103) are different as shown in table (5).
Table 5

*Effects of Reynolds Number on Two Fiber Sedimentation*

<table>
<thead>
<tr>
<th>Case No.</th>
<th>Particle Shape</th>
<th>Reynolds Number</th>
<th>Young’s modulus</th>
<th>Rigidity</th>
<th>Elasto - gravitation numbers</th>
<th>Settling velocity</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>cuboid</td>
<td>1.9</td>
<td>0.5</td>
<td>0.486</td>
<td>2.88</td>
<td>0.0019</td>
</tr>
<tr>
<td>2</td>
<td>cuboid</td>
<td>35</td>
<td>0.5</td>
<td>0.486</td>
<td>0.072</td>
<td>0.034</td>
</tr>
<tr>
<td>3</td>
<td>cuboid</td>
<td>71</td>
<td>0.5</td>
<td>0.486</td>
<td>0.024</td>
<td>0.07</td>
</tr>
<tr>
<td>4</td>
<td>cuboid</td>
<td>103</td>
<td>0.5</td>
<td>0.486</td>
<td>0.014</td>
<td>0.1</td>
</tr>
</tbody>
</table>

In all cases, same Rigidty have been used (EI=0.486) by fixed the young's modulus (E=0.5). All fibers settle down in a viscous fluid (ν = 0.04). It is observed that the fibers with higher Reynolds number settle faster than the fibers with lower Reynolds number as shown in figures (26,27,28,29). By looking into the velocity field in the fluid, which is easy to visualize how increasing Reynolds number increases the sedimentation velocities.
Figure 26: The trajectories of vertical velocity $V_z$ with $Re = 1.9$

Figure 27: The trajectories of vertical velocity $V_z$ with $Re = 35$
Figure 28: The trajectories of vertical velocity $V_z$ with $Re = 71$

Figure 29: The trajectories of vertical velocity $V_z$ with $Re = 103$
Figure (30) displays a comparison of the curvature index between the two cases of Re=1.9 and Re=35. It is shown that the deformation of case1 with Re=1.9 is smaller than the deformation of case2 with Re=35. Thus, deformation increases as the Reynold number increases.

Figure 30: Comparison of the curvature index between the two cases of Re=1.9 and Re=35
Figure 31: The angular distribution function of fibers segments, a) Re=1.9, b) Re=35, c) Re=71, d) Re=103

The angular distribution function is computed for the four cases with different Reynolds numbers and compared in figure (31). It shows that fibers are preferentially oriented horizontally. However, the multi-particle interaction causes some fiber orientation deviate from the horizontal direction. The results demonstrate that the low Reynolds number case has a larger probability to be oriented in horizontal direction than the higher Reynolds number.
6.2.4. Effects of Distance Between Two Fibers Sedimentation

Cases (1, 2, 3) measure the effect of three initial distances between two fibers. In all cases, same Rigidity have been used (EI=0.029) by fixed the young's modulus (E=0.03). All fibers settle down in a viscous fluid (v = 0.04). Figures (32,33,34) show the settling velocities of two rectangular fibers at different distance between the two fibers with fixed all other conditions. It clearly shows that the settling velocity decrease rapidly when the distance between two fibers increases. In figure (35-a), the two fibers are close each other (10 lattice units). The weak effect of the leading particle is clearly observed. This may tell that the drafting, kissing and tumbling happens and are repeated for many times. In figure (35-b,c) shows that the weak generated by the leading particle is reduced. The weak is not strong enough to trap the trailing particle, so the number of drafting, kissing and tumbling is reduced, thus the settling velocities of two rectangular fibers will decrease also.

<table>
<thead>
<tr>
<th>Case No.</th>
<th>Particle Shape</th>
<th>Distance</th>
<th>Reynolds Number</th>
<th>Young’s modulus</th>
<th>Density</th>
<th>Elasto-gravitation numbers</th>
<th>Settling velocity</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>cuboid</td>
<td>10</td>
<td>37.9</td>
<td>0.03</td>
<td>1.2</td>
<td>0.0043</td>
<td>0.038</td>
</tr>
<tr>
<td>2</td>
<td>cuboid</td>
<td>20</td>
<td>35.8</td>
<td>0.03</td>
<td>1.2</td>
<td>0.0043</td>
<td>0.035</td>
</tr>
<tr>
<td>3</td>
<td>cuboid</td>
<td>30</td>
<td>33.8</td>
<td>0.03</td>
<td>1.2</td>
<td>0.0043</td>
<td>0.033</td>
</tr>
</tbody>
</table>
Figure 32: The trajectories of vertical velocity $V_z$ with 10 lattice units distance between the two particles.

Figure 33: The trajectories of vertical velocity $V_z$ with 20 lattice units distance between the two particles.
Figure 34: The trajectories of vertical velocity $V_z$ with 30 lattice units distance between the two particles.
Figure 35: Sedimentation of two rectangular fibers with different distance between the two fibers. a) 10 lattice units, b) 20 lattice units, c) 30 lattice units.
Figure 36: The angular distribution function of fibers segments with different distance between the two fibers a) 10 lattice units, b) 20 lattice units, c) 30 lattice units
In figure (36), the angular distribution function is calculated for fibers segments with different distance between the two fibers. It is found that increasing the distance between the two particles increase fiber orientation deviation from the horizontal direction and therefore, increase the probability to be oriented in horizontal direction.

Figure 37: Comparison of the curvature index between different distance between the two particles, 10, 20, and 30

Figure (37) displayed comparison of the curvature index between different initial distance. The results showed that the deformation increases by increase the initial distance. However, a large distance takes a longer time for the particle to be deformed.

6.2.5. Effects of Particle Dimensions of Two Fibers

To investigate the effects of fiber size and aspect ratio on the sedimentation process, we conduct simulations with different dimension and aspect ratio as shown in table (7).
Table 7

*Effects of Particle Dimensions of Two Fibers Sedimentation*

<table>
<thead>
<tr>
<th>Case No.</th>
<th>Particle Shape</th>
<th>Particle Dimension</th>
<th>Aspect Ratio</th>
<th>Reynolds Number</th>
<th>Rigidity</th>
<th>Settling velocity</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Cuboid</td>
<td>5,5,41</td>
<td>8.2</td>
<td>26.65</td>
<td>0.0149</td>
<td>0.026</td>
</tr>
<tr>
<td>2</td>
<td>Cuboid</td>
<td>7,7,41</td>
<td>5.857</td>
<td>35.875</td>
<td>0.029</td>
<td>0.035</td>
</tr>
<tr>
<td>3</td>
<td>Cuboid</td>
<td>9,9,41</td>
<td>4.555</td>
<td>45.1</td>
<td>0.048</td>
<td>0.044</td>
</tr>
</tbody>
</table>

In cases 1, 2 and 3, same particles length with variety cross section have been used. The other properties (density, viscosity, young's models, epsilon ... etc.) were fixed. The trajectories of vertical velocity $V_z$ are plotted as function of time as shown in figures (38,39,40) for the three cases. As expected, the settling fibers velocity increases by increasing fiber dimensions due to the fact that the larger particle settles more quickly than the smaller one, figure (41).
Figure 38: The trajectories of vertical velocity $V_z$ with particle dimension 5,5,41

Figure 39: The trajectories of vertical velocity $V_z$ with particle dimension (7,7,41)
Figure 40: The trajectories of vertical velocity $V_z$ with particle dimension $(9,9,41)$

Figure 41: A comparison between three different cases of sedimentation of two particles with different particles dimensions a) $P=5,5,41$, b) $P=7,7,41$, c) $P=9,9,41$
In figure (41), a comparison of the curvature index between different particles dimension is displayed. It is found that the deformation increases by decreasing particle aspect ratio.

The angular distribution function of fibers segments with different particle aspect ratio are displayed in figure (42). It has been found that the large particles dimension has larger probability to be oriented in horizontal direction than the small particles.
Figure 42: Comparison of the curvature index between different particles dimension a. (5,5,41), b. (7,7,41) and c. (9,9,41)
Figure 43: The angular distribution function of fibers segments with different particles dimension a. (5,5,41), b. (7,7,41) and c. (9,9,41)
6.2.6. Effects of Particle Aspect Ratio of Two Fibers Sedimentation

To assess the impact of aspect ratio on the dynamical behavior of fibers simulation, we conduct simulation of three cases with three different aspect ratio ($\kappa=3$, $\kappa=5.857$, $\kappa=7.286$). The results (figures 44,45,46) show that the decrease of the aspect ratio will shorten the time for the two particles to undergo the DKT process, while the increase of aspect ratio can enhance the occurrence of the repeated DKT process. However, aspect ratio has little impact on fibers settling velocity as shown in figure (47).

Table 8

*Effects of Particle Aspect Ratio of Two Fibers Sedimentation*

<table>
<thead>
<tr>
<th>Case No.</th>
<th>Particle Shape</th>
<th>Particle Dimension</th>
<th>Aspect Ratio</th>
<th>Reynolds Number</th>
<th>Rigidity</th>
<th>Settling velocity</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>cuboid</td>
<td>7,7,21</td>
<td>3</td>
<td>16.275</td>
<td>0.111</td>
<td>0.031</td>
</tr>
<tr>
<td>2</td>
<td>cuboid</td>
<td>7,7,41</td>
<td>5.857</td>
<td>35.875</td>
<td>0.029</td>
<td>0.035</td>
</tr>
<tr>
<td>3</td>
<td>cuboid</td>
<td>7,7,51</td>
<td>7.286</td>
<td>45.9</td>
<td>0.0188</td>
<td>0.036</td>
</tr>
</tbody>
</table>
Figure 44: The trajectories of vertical velocity $V_z$ with aspect ratio 3, ($P=7,7,21$)

Figure 45: The trajectories of vertical velocity $V_z$ with aspect ratio 5.857 ($P=7,7,41$)
Figure 46: The trajectories of vertical velocity $V_z$ with aspect ratio 7.286, (P=7,7,51)

Figure 47: A comparison between three different cases of sedimentation of two particles with different aspect ratio a) $\kappa=3$ , b) $\kappa=5.857$ ,c) $\kappa=7.286$
Figure 48: Comparison of the curvature index between different particles aspect ratio, a) \( \kappa=3 \), b) \( \kappa=5.857 \) and c) \( \kappa=7.286 \)
Figure 49: The angular distribution function of fibers segments with different particles aspect ratio a) $\kappa=3$, b) $\kappa=5.857$ and c) $\kappa=7.286$
In figure (48) displayed a comparison of the curvature index between different particles aspect ratio. It is show that the deformation increase by increasing particles aspect ratio.

In figure (49), the angular distribution function of fibers segments with different particles aspect ratio are displayed. It is found that the increase the aspect ratio will reduce the particles' probability to be oriented in horizontal direction.

6.3. Sedimentation of Two Cylinder Fibers

To investigate flexibility effect on two cylinders’ fiber sedimenting in vertical rectangular channel, four simulations are carried out in the same conditions of fiber dimensions and fluid viscosity, except fiber flexural. Rigidity are varied at four different levels \( EI = 0.026, EI = 0.642, EI = 0.053 \) and \( EI = 0.696 \) respectively. Same simulation box of 60 x 160 x 900 lattice units was used. In this scale, the length of the fiber is \( L = 41 \) lattice units, and the diameter of the fiber is \( d = 7 \) lattice units, which gives the fiber an aspect ratio of \( \kappa = 5.857 \).

Table 9

\textit{Sedimentation of Two Cylinder Fibers}

<table>
<thead>
<tr>
<th>Case No.</th>
<th>Particle Shape</th>
<th>Density</th>
<th>Reynolds Number</th>
<th>Young’s modulus</th>
<th>Rigidity</th>
<th>Elasto-gravitation numbers</th>
<th>Settling velocity</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>cylinder</td>
<td>1.4</td>
<td>53.3</td>
<td>0.05</td>
<td>0.026</td>
<td>0.002</td>
<td>0.052</td>
</tr>
<tr>
<td>2</td>
<td>cylinder</td>
<td>1.4</td>
<td>50</td>
<td>1.2</td>
<td>0.047</td>
<td>0.642</td>
<td>0.046</td>
</tr>
<tr>
<td>3</td>
<td>cylinder</td>
<td>1.6</td>
<td>68.4</td>
<td>0.1</td>
<td>0.0026</td>
<td>0.053</td>
<td>0.066</td>
</tr>
<tr>
<td>4</td>
<td>cylinder</td>
<td>1.6</td>
<td>64</td>
<td>1.3</td>
<td>0.034</td>
<td>0.696</td>
<td>0.062</td>
</tr>
</tbody>
</table>
Figure 50: The trajectories of vertical velocity $V_z$ of cylinder fibers (Flexible Particle) at $Re=53.3$.

Figure 51: The trajectories of vertical velocity $V_z$ of cylinder fibers (Rigid Particles) at $Re=50$.
The trajectories of vertical velocity $V_z$ of the flexible and rigid particles are plotted as a function of time step. In the Figures (50, 51), we can see that settling vertical velocities of the rigid particles (case 2) affected slightly compared to the flexible particles (case 1). In the flexible case, drafting, kissing and tumbling process is repeated more than the rigid case. We can indicate that the increasing in flexibility will help the two cylinder particles to touch and change their position more. The flexibility allows the particle sliding faster. Thus, the sedimentation of flexible cylinder particles faster than the rigid cylinder particles because of increasing of the wake flow.

Figure 52: The trajectories of vertical velocity $V_z$ of cylinder fibers (Flexible Particles) at Re=68.4
Figure 53: The trajectories of vertical velocity $V_z$ of cylinder fibers (Rigid Particles) at Re=64.

In the cases 3 and 4, the Reynolds number increased by increase particle density to be 1.6. Other kinematic parameters are kept the same. (aspect ratio, viscosity, epsilon ... etc.). The trajectories of vertical velocity $V_z$ of the flexible and rigid particles are shows in Figures (52, 53). the flexible fibers still settling faster than the rigid particle and have higher number of Drafting–Kissing– Tumbling (DKT) circle.
CHAPTER VII
DISCUSSION AND CONCLUSION

The behavior of flexible fibers has been accurately simulated in low and moderate Reynolds number. Simulations of fibers by using lattice Boltzmann methods demonstrated that the method can reproduce known dynamical behavior of both rigid and flexible fibers. The lattice Boltzmann and lattice spring methods have been employed to stimulate the behavior of flexible fibers and to measure the sedimentation velocity. In the simulations, flexibility, Reynolds numbers, density, fibers shape and aspect ratio are varied. Many cases of single and two particles have been run.

For the sedimentation of single particle, it is shown that deformation due to flexibility plays an important role in settle velocity. Thus, fibers deformations increase by increase its flexibility. The investigate of effect particles Reynolds number shows that particle settling velocity increases with increasing particle Reynolds number. The fibers with high Reynolds numbers can be deformed more easily and fitted more conformably with the streamlines than lower Reynolds number' fibers. In other hand, the elastic gravitational force is inversely proportional with Reynolds number due to increase particle density which leads to increase gravitation force.

It has been found that the sedimentation behavior of two fibers is different from a single fiber. The Drafting, kissing and tumbling (DKT) are observed in a two-fiber system. The Drafting occurs when the trailing fiber move into the wake area of the leading fiber. The trailing and leading fibers contact each other in the kissing stage. Tumbling occurs when the trailing particle becomes the leading one. The number of Drafting Kissing
tumbling process of two fibers is influenced strongly by the particle flexibility. The simulations demonstrate that the settling velocity of fibers suspension increases as the fiber flexibility increase. The number of Drafting–Kissing–Tumbling (DKT) process increases as flexibility increase. The results of the curl index shown that fibers deformations increase by increase its flexibility. A flexible fiber can be deformed more easily and fitted more conformably with the streamlines than a rigid fiber. That, the settling velocity increases as the fiber flexibility increases. The results demonstrate that the stiff fibers have a larger probability to be oriented in horizontal direction than the flexible fibers due to their bending or shape deformation.

The study investigates the effect of Reynold number on two particle sedimentation. The results demonstrate that as the fibers Reynold numbers increase, the settling velocity increases also. The deformation increases as the Reynold number increases. The results show that the low Reynolds number case has a larger probability to be oriented in horizontal direction than the higher Reynolds number.

The study shows that the settling velocity decrease rapidly when the distance between two fibers increases. It is found that increasing the distance between the two particles increase fiber orientation deviation from the horizontal direction and therefore, increase the probability to be oriented in horizontal direction. It is found, also, that the deformation increases by increase the initial distance, however, a large distance takes a longer time for the particle to be deformed.
It is found that the decrease of the aspect ratio will shorten the time for the two particles to undergo the DKT process, while the increase of aspect ratio can enhance the occurrence of the repeated DKT process. However, aspect ratio has little impact on fibers settling velocity. The initial distance between two fibers have little impact on fiber settling velocity. A larger initial distance increases the DKT cycling time.

The study investigates the behavior of sedimentation of two cylinder fibers. The results indicate that the increasing in flexibility will help the two cylinder particles to touch and change their position more. The flexibility allows the particle sliding faster. Thus, the flexible fibers settling faster than the rigid particle and have higher number of Drafting–Kissing–Tumbling (DKT) circle.

This work demonstrate that the lattice Boltzmann method could be accurately used to simulate the motion of flexible fibers.
REFERENCES


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APPENDIX

NOMENCLATURE

1. $\tau$ -- single relaxation time
2. $\theta_L$ -- leading edge angle
3. $\vec{c}_i$ -- semi-axis vector of the wing segment in the body-fixed coordinate system
4. $\vec{F}^h_i$ -- total hydrodynamic force on solid particle $i$
5. $\vec{F}_i$ -- total force on segment $i$
6. $\vec{R}_i$ -- position vector of the mass center of solid segment $i$
7. $f^\alpha_\sigma(\vec{x},t)$ -- fluid particle distribution function
8. $f^{\text{eq}}_\sigma(\vec{x},t)$ -- equilibrium distribution function
9. $\Delta\theta_L$ -- leading edge deflection angle
10. $\delta t$ -- length of time step
11. $\epsilon$ -- Knudsen number
12. $\kappa$ -- reduced frequency
13. $\nu$ -- kinematic viscosity
14. $\omega$ -- flapping angular velocity
15. $\omega^*$ -- Normalized frequency
16. $\omega_0$ -- Nature frequency
17. $\omega_\sigma$ -- weight coefficient
18. \( \rho_f \) -- fluid density

19. \( \rho_s \) -- wing density

20. \( \sigma \) -- direction number of the particle discrete velocity

21. \( \theta \) -- pitch angle

22. \( \Theta_i \) -- bending angle between the \( i \)th and \( (i+1) \)th segment

23. \( \alpha_t \) -- trailing edge angle

24. \( \tilde{e}_\sigma \) -- particles discrete velocity

25. \( \vec{C}_i^+ \) -- vector from the mass center of the segment \( i \) to the joint

26. \( F \) -- hydrodynamic force

27. \( \ddot{u} \) -- Fluid velocity

28. \( J \) -- position vector of the fluid boundary node

29. \( r^b \) -- position vector of the solid boundary node

30. \( E \) -- Young’s modulus

31. \( EI_i \) -- bending flexural rigidity

32. \( f \) -- flapping frequency

33. \( F_f \) -- non-dimensional hydrodynamic force per unit chord length

34. \( f_p \) -- power efficiency

35. \( F_y \) -- total hydrodynamic force in the y-direction

36. \( F_z \) -- total hydrodynamic force in the z-direction

37. \( h \) -- wing thickness

38. \( M \) -- mass of segment
39. $\dot{\theta}_z$ -- pitch angular velocity

40. $P$ -- power input coefficient

41. $p$ -- pressure

42. $Re$ -- Reynolds number

43. $s$ -- span length

44. $t_c$ -- time after fluid particle collision

45. $t_0$ -- short time scale

46. $t_l$ -- long time scale

47. $U_0$ -- reference velocity

74. $\tilde{U}_c$ -- velocity of the mass center of solid segment