Study of Fluid Forces and Heat Transfer on Non-Spherical Particles in Assembly Using Particle Resolved Simulation

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Dissertation submitted to the faculty of the Virginia Polytechnic Institute and State University in partial fulfillment of the requirements for the degree of Doctor of Philosophy in Mechanical Engineering

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Abstract

Gas-solid flow is fundamental to many industrial processes. Extensive experimental and numerical studies have been devoted to understand the interphase momentum and heat transfer in these systems. Most of the studies have focused on spherical particle shapes, however, in most natural and industrial processes, the particle shape is seldom spherical. In fact, particle shape is one of the important parameters that can have a significant impact on momentum, heat and mass transfer, which are fundamental to all processes. In this study particle-resolved simulations are performed to study momentum and heat transfer in flow through a fixed random assembly of ellipsoidal particles with sphericity ($\psi = 0.887$). The incompressible Navier-Stokes equations are solved using the Immersed Boundary Method (IBM). A Framework for generating particle assembly is developed using physics engine—PhysX. High-order boundary conditions are developed for immersed boundary method to resolve the heat transfer in the vicinity of fluid/particle boundary with better accuracy. A complete framework using particle-resolved simulation study assembly of particles with any shape is developed. The drag force of spherical particles and ellipsoidal particles are investigated. Available correlations are evaluated based on simulation results and recommendations are made regarding the best combinations. The heat transfer in assembly of ellipsoidal particle is investigated, and a correlation is proposed for the particle shape studied. The lift force, lateral force and torque of ellipsoidal particles in assembly and their variations are quantitatively presented and it is shown that under certain conditions these forces and torques cannot be neglected as is done in the larger literature.
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General Audience Abstract

Gas-solid flow is fundamental to many industrial processes such as pollution control, CO2 capture, biomass gasification, chemical reactors, sprays, pneumatic conveying, etc. Extensive experimental and numerical studies have been devoted to understand the interphase momentum and heat transfer in these systems. Most of the studies have focused on spherical particle shapes, however, in most natural and industrial processes, the particle shape is seldom spherical. In fact, particle shape is one of the important parameters that can have a significant impact on momentum, heat and mass transfer, which are fundamental to all processes. In this study particle-resolved simulations are performed to study momentum and heat transfer in flow through a fixed random assembly of ellipsoidal particles. A Framework for generating particle assembly is developed using physics engine—PhysX. A complete framework using particle-resolved simulation study assembly of particles with any shape is developed. The drag force of spherical particles and ellipsoidal particles are investigated. Available correlations are evaluated based on simulation results and recommendations are made regarding the best combinations. The heat transfer in assembly of ellipsoidal particle is investigated, and a correlation is proposed for the particle shape studied. The lift force, lateral force and torque of ellipsoidal particles in assembly and their variations are quantitatively presented and it is shown that under certain conditions these forces and torques cannot be neglected as is done in the larger literature. The framework developed in this work can be used to study the heat and momentum transfer in flow with spherical and non-spherical particles. With data collected using this method, more accurate drag and heat transfer models can be developed for fluid-particle system.
Dedication

Dedicated to Mom and Dad

It's impossible to thank you adequately for everything you've done.
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Chapter 1

Introduction

Gas-solid flow is fundamental to many industrial processes such as pollution control, CO2 capture, biomass gasification, chemical reactors, sprays, pneumatic conveying, etc. Extensive experimental and numerical studies have been devoted to understand the interphase momentum and heat transfer in such flows during the last several decades. Most of the studies have focused on spherical particle shapes to simplify the challenge of understanding the flow and particle interactions. However, in most natural and industrial processes, the particle shape is seldom spherical. In fact, particle shape is one of the important parameters that can have a significant impact on momentum, heat and mass transfer, which are fundamental to all processes. Although these effects of particle shape have already been widely recognized, only a few studies have been carried out to quantify them.

Typically, experimental measurements are quite challenging because of the abrasive and opaque environment encountered in many of the flow systems. Thus, computational modeling plays an important role to aid the fundamental understanding of inter-phase interactions. The widely used computational techniques for simulating particulate flows can be classified into three categories: (1) Two-Fluid model (TFM) in which particles are treated in the continuum as an interpenetrating medium with the fluid. (2) Discrete Element method (DEM) in which fluid motion is described by the Navier-Stokes equation while the particles are treated as discrete entities in a Lagrangian framework using Newton’s second law to estimate particle acceleration and position and conservation of angular momentum to describe its angular rotation and position. The essentials of DEM include a collision
model to calculate collision forces, and models for drag forces and other unsteady force terms to model the forces experienced by the particle. (3) Particle-Resolved simulations (PRS) in which the fluid and particulate phases are governing by the Navier-Stokes equation and the Lagrangian equations of motion, respectively. In this method, no-slip boundary condition is set at the fluid-particle interface and the fluid force acting on particle is calculated based on the resolved fluid field. Thus, no empirical closure is needed in this method. In the simulation hierarchy from PRS-to-DEM-to-TFM, computational complexity reduces but so does the increasing dependence on modelling the complex interactions between the two phases. In both DEM and TFM drag correlations and heat transfer correlations play a critical role in the dynamics of the system. However, even for the most essential and widely studied correlation: drag models for spherical particles, there are significant disagreements between correlations. Figure 1.1 shows the snapshots of flow patterns at different time stamps from a DEM simulation of a fluidized bed [1]. In this method, the motion of each individual solid particle is described by Newton’s second law:

$$m \frac{du}{dt} = F_G + F_C + F_{F-P}$$  \hspace{1cm} \text{Equation 1.1}$$

Where $F_G$ denotes the gravity force, $F_C$ denotes the contact force due to particle-particle collision, and $F_{F-P}$ denotes the fluid-particle interaction force. $F_{F-P}$ can be obtained by:

$$F_{F-P} = F_H + F_{AM} + F_D$$  \hspace{1cm} \text{Equation 1.2}$$

$F_H$ denotes the history force (also referred as Basset force), $F_{AM}$ denotes the added mass force. Both $F_H$ and $F_{AM}$ represent unsteady force generated by the non-stationary motion of particle and fluid. $F_D$ is the steady fluid drag force in uniform flow. The five simulations have the same numerical setup, and only the drag model [2–5] for predicting the $F_D$ is different. The snapshots show that the flow structure is highly affected by the drag model: simulation (d) and (e) have significant higher bed height than simulation (a) to (c). For non-spherical particles, the developing of such drag models is
much more challenging. Moreover, due to the non-spherical particle shape, secondary forces (forces normal to the particle-fluid relative velocity) and fluid torque are also introduced. For isolated single non-spherical particles, there are limited number of general drag force correlations available. Lift and torque correlations have been proposed for certain particle shapes, but no general correlation is available. For particles in assembly, limited number of studies have been carried out to predict the drag force, while markedly scarce information is available for predicting secondary forces and torque. Compared to momentum transfer, the development of heat transfer correlations for non-spherical particles is even worse. To the author’s knowledge, there are no heat transfer correlations that have been proposed for non-spherical particle in assembly.

**Figure 1.1. Fluidized bed with different drag law, from paper[1]**
Because of the high fidelity and independence from empirical modeling, Particle-Resolved simulations are used in this research to study the momentum and heat transfer in fluid with non-spherical particles. In doing so, there are numerous challenges:

- An efficient and robust framework is necessary to generate the random assemblies of non-spherical particles.
- An accurate method to resolve the momentum and heat transfer between different fluid and solid.
- Handling and processing of large amounts of data.

The main objective of this work is to develop the numerical methods necessary to study the momentum and heat transfer in particle assemblies of any shape. The following are the major research contributions as part of the current work:

- Framework for generating particle assembly is developed using physics engine—PhysX.
- High-order boundary conditions are developed for immersed boundary method to resolve the heat transfer in the vicinity of fluid/particle boundary with better accuracy.
- A complete framework using particle-resolved simulation study assembly of particles with any shape is developed, shown in Figure 1.2.
- The steady fluid drag force ($F_D$ in Equation 1.2) of spherical particles and ellipsoid particles is investigated. Available correlations are evaluated based on simulation results and recommendations are made regarding the best combinations.
- The heat transfer in assembly of ellipsoid particle is investigated, and a correlation is proposed for the particle shape studied.
The lift force, lateral force and torque of ellipsoid particles in assembly and their variations are quantitatively presented and it is shown that under certain conditions these forces and torques cannot be neglected as is done in the larger literature.

**Figure 1.2: Framework developed for simulating non-spherical particle assembly**

This thesis is organized as follows:

- In chapter 2, momentum transfer with spherical particles and ellipsoidal particles is studied. Numerical techniques, method for generating the random assembly of non-spherical particles, and the simulation model are presented with details.

- In chapter 3, heat transfer in fluid with ellipsoidal particles is studied. Nusselt number of assembly of spherical particles predicted by the current model is compared with widely used correlations and previous particle resolved simulation data. For assembly of ellipsoidal particles, a new Nusselt number correlation is proposed based on simulation data.
In chapter 4, mean and variation of drag force, lift force, lateral force and torque on ellipsoidal particle in assembly are investigated. The mean value of forces and torque and their variation are discussed.

The work performed as part of this dissertation has resulted in peer-review journal publications and the details are as follows:


Chapter 2
Evaluation of Drag Correlations Using Particle Resolved Simulations of Spheres and Ellipsoids in Assembly

2.1 Abstract

Particle-resolved simulations are performed to study the momentum transfer in flow through fixed random assembly of non-spherical particles. Ellipsoidal particles with sphericity ($\psi = 0.887$) are investigated in a periodic cubic domain to simulate an infinite assembly. The incompressible Navier-Stokes equations are solved using the Immersed Boundary Method (IBM). Pressure and viscous force on each particle are calculated based on the resolved flow field. Flow through an assembly of spherical particles is tested, and predicted drag forces are compared with previous particle resolved simulation results to validate the current framework. The assembly of ellipsoidal particles is simulated for solid fraction between 0.1 to 0.35 using 191 to 669 particles, respectively, at low to moderate Reynolds numbers ($10 \leq Re \leq 200$). The simulation results show that the drag force of ellipsoidal particles is 15% to 35% larger than equal volume spherical particles. Widely used drag force correlations are evaluated based on the current simulation results. The comparisons show that for ellipsoidal particles over the range of parameters investigated in the present study, the combination of Tenneti et al.’s correlation with Holzer’s single non-spherical particle drag model has the best performance with an average difference of 7.15%.
2.2 **Keywords**

Particle resolved simulation; non-spherical particle; ellipsoid; drag correlation; immersed boundary method.

2.3 **Introduction**

Gas-solid flow is fundamental to many industrial processes such as pollution control, CO2 capture, biomass gasification, chemical reactors, sprays, pneumatic conveying, etc. Extensive experimental and numerical studies have been devoted to understand the interphase momentum transfer in such flows during the last several decades. Most of the studies have focused on spherical particle shapes to simplify the challenge of understanding the flow and particle characteristics. However in most natural and industrial processes, the particle shape is seldom spherical. In fact, particle shape is one of the important parameters that can have a significant impact on momentum, heat and mass transfer, which are fundamental to all processes. Although these effects of particle shape have already been widely recognized, only a few studies have been carried out to quantity them.

Most research on drag coefficient for non-spherical particle have focused on a single isolated particle. Yow et al. [6] collected experimental data of drag coefficient for a wide range of shapes including spheres, cube octahedrons, octahedrons, cubes, tetrahedrons, discs, cylinders, rectangular parallelepipeds and others. By studying the variation of drag coefficient against Reynolds number for different non-spherical particles, they showed that as the sphericity decreased, the drag coefficient increased significantly. Consequently, several drag correlations have been developed based on experimental data, using particle shape and Reynolds number as parameters. Chhabra et al. [7] studied correlations for estimating the drag coefficient of non-spherical particles in incompressible viscous fluids. 1900 experimental data points from 19 independent studies were used to evaluate the...
accuracy of five correlations, including those proposed by Haider and Levenspiel [8], Ganser [9], Chien [10], Hartman et al. [11] and Swamee and Ojha [12]. They found that the correlation developed by Ganser, which uses the equivalent spherical diameter and the sphericity as the particle shape parameters, performed the best. The average error from this method was 16%, though the maximum error was as high as 180%. Holzer and Sommerfeld [13] developed a general drag correlation which depends on particle sphericity, Reynolds number, and particle orientation. Comparing to 2061 experimental data points, they showed that the new correlation had a mean relative deviation of 14.1%. After performing experimental measurements of the terminal velocities of irregular particles falling in fluids, Dioguardi and Mele [14] proposed a drag correlation using sphericity and circularity as shape factors. They found the new correlation is able to predict the terminal velocity with about 11% error when the Reynolds number is known. Using a similar experimental setup, Dioguardi et al. [15] proposed another shape-dependent drag coefficient and integrated it into the multiphase code MFIX-DEM. Bagheri and Bonadonana [16] recently proposed a general model for prediction drag coefficient for non-spherical particles for Reynolds number up to $3 \times 10^5$ based on experimental data. Instead of using the sphericity, this new correlation uses two shape factors based on the particle flatness and elongation, and diameter to quantify the shape of the particles. The authors state that the new correlation has an average error of ~10%, which is significantly lower than existing correlations.

Compared to the rich database and correlations available for drag of an isolated particle, only a few studies focusing on drag coefficient of packed non-spherical particles have been carried out. Nemec and Levec [17] demonstrated that the original Ergun equation [3] is only able to predict the pressure drop in flow over spherical particles, whereas it systematically under-predicts the pressure drop in flow over non-spherical particles. They proposed that the dimensionless form of the Ergun equation, developed by Niven [18] with two constant factors, which only vary for different particle shapes, should be used for non-spherical particles. They conclude that with their modifications, the
Ergun equation is able to predict pressure drop in flow through a packed bed of certain non-spherical particles within 10% error. However, there is no correlation to calculate the constants for arbitrary particle shapes, leaving that determination to experiments or particle resolved simulations. Moreover, the original Ergun equation significantly over-predicts the average drag force at low solid volume fractions [19], and hence the modified equation applied to a dilute system of non-spherical particles has not been validated. Machač and Dolejš [20] investigated the pressure drop in flow through a random fixed bed of non-spherical particles. They suggested that a ‘bed factor’ which contains the information of the non-spherical particle surface area is needed to accurately predict the pressure drop. Hua et al[21] studied the combined Ganser and Ergun correlations and modified Syamlal and O’Brien drag models in Eulerian-Eulerian CFD framework for irregular shape in dense gas-solid fluidized beds. Dorai et al. [22] examined the local packing structure of fixed bed reactors made of cylindrical pellets packed in cylindrical tubes. They found that the local packing structure (particle orientation) is strongly affected by the particle size distribution. Zhou et al. [23] studied packed ellipsoidal particles in a fluidized bed using CFD-DEM simulations. The drag model developed by Holzer et al. [13] was used for the ellipsoids. They concluded that the accuracy and applicability of current correlations is questionable, and a general and reliable correlation to determine fluid drag on non-spherical particles is urgently needed. Vollmari et al. [24] investigated the pressure drop in packing of arbitrary shaped particles using CFD-DEM and experiment. Based on experimental measurements, they suggested that particle drag in DEM simulations should be calculated combining the correlations developed by Holzer et al. [13] and De Felice [25]. They recommend fully resolved simulations to understand the effects of inhomogeneous packing on fluid flow structure introduced by the non-spherical particle shape.

All these studies demonstrate that further investigation is needed to have a better understanding of flow through an assembly of non-spherical particles. Therefore, in this study,
particle-resolved simulations are carried out to investigate momentum transfer for a random assembly of non-spherical particles. In this approach, fluid force on each particle is calculated by resolving the flow field around each individual particle. Ellipsoidal particles with aspect ratio of 2.5 are used and the particle-fluid boundaries are resolved using an Immersed Boundary Method (IBM). The objectives of the current study are: (1) validate the current particle resolved simulation framework by comparing results for flow through spherical particle assemblies to existing drag correlations; (2) simulate flow through an assembly of ellipsoids and extract the drag force; (3) evaluate the performance of existing drag correlations for the non-spherical particles.

2.4 Numerical method

All simulations are performed using an in-house code – Generalized Incompressible Direct and Large Eddy Simulation of Turbulence (GenIDLEST). The details of the framework and methodology used in GenIDLEST can be found in Tafti [26] and Tafti [27]. In this section, the relevant governing equations and the modified treatments of the governing equations under fully-developed flow conditions are presented along with some details of the Immersed Boundary Method [28]. GenIDLEST with immersed boundary method has been successfully applied to oscillating cylinders [28], turbine cooling passage heat transfer [29], and fluid structure interactions problems [30].

2.4.1 Governing Equations and Numerical Technique

The non-dimensional form of the Navier-Stokes equations for incompressible flow are as follows:

Continuity:
\[
\frac{\partial u_i}{\partial x_i} = 0
\]  \hspace{1cm} \text{Equation 2.1}

Momentum:
\[
\frac{\partial u_i}{\partial t} + \frac{\partial(u_i u_j)}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{1}{Re_{ref}} \left( \frac{\partial^2 u_i}{\partial x_j \partial x_j} \right)
\]  \hspace{1cm} \text{Equation 2.2}

where the non-dimensionalizations are:
\[
x_i = \frac{x_i}{L_{ref}}; u_i = \frac{u_i}{u_{ref}}; t = \frac{t^* u_{ref}}{L_{ref}}; P = \frac{p^* - p_{ref}^*}{\rho_{ref} u_{ref}^2}; Re_{ref} = \frac{\rho_{ref} u_{ref} L_{ref}}{\mu_{ref}}
\]

The above governing equations are transformed to generalized coordinates, and discretized in a conservative finite-volume formulation using a second-order central (SOC) difference scheme on a non-staggered grid topology [31]. Cartesian velocities, pressure and temperature are calculated and stored at the cell center, whereas fluxes are calculated and stored at cell faces. A projection method using second order predictor-corrector steps is used for the time integration of the continuity and momentum equations. In the predictor step, an intermediate velocity field is calculated; and in the corrector step, an updated divergence free velocity is calculated at the new time-step by solving a pressure-Poisson equation.

2.4.2 Fully developed calculations

The computational domain consists of a three-dimensional periodic box representing an unbounded particle assembly. Flow is induced along the x-direction by applying a constant mean pressure gradient to balance the form and friction losses, and the total pressure is expressed in terms of the mean pressure and a fluctuating or periodic component as shown in Equation 2.3.
\[
P(\bar{x}, t) = -\beta \cdot x + p(\bar{x}, t)
\]  \hspace{1cm} \text{Equation 2.3}
where $\beta$ is a constant. Because the applied pressure gradient will balance the form and friction losses when the flow reaches a steady state, the actual value used for $\beta$ is not of any consequence to the calculated forces as long as the mean Reynolds number obtained from the simulation is the same.

With the unchanged continuity equation, the momentum equation can be written as:

$$\frac{\partial u_i}{\partial t} + \frac{\partial (u_j u_i)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{1}{Re_{ref}} \left( \frac{\partial^2 u_i}{\partial x_j \partial x_j} \right) + \beta \vec{e}_x \quad \text{Equation 2.4}$$

The $\beta \vec{e}_x$ in Equation 4 is the mean applied pressure gradient source term, which balances the mean form and friction losses in the flow direction. The detailed procedure used can be found in Patankar [32] and Zhang et al. [33].

2.4.3 IBM

The immersed boundary method (IBM) used in this paper is an indirect forcing sharp interface approach. This method is an extension of a scheme originally proposed by Gilmanov and Sotiropoulos [34], and has been modified to fit the generalized coordinate system and non-staggered grid framework of GenIDLEST. In this method, the governing equations are solved without modification for the computational grid in the fluid domain. Special treatment is only applied to the first layer of the fluid nodes (fluid IB nodes) next to the immersed boundary. The major steps of this method are summarized below. The details can be found in Nagendra et al. [28].

1. Definition of surface grid

The immersed boundary is the fluid/solid interface which is provided as input in a discretized form of an unstructured surface mesh. Each of the immersed boundary elements has information of surface normal, area, and location with respect to the fixed background fluid mesh.

2. Node identification
By employing a search-locate and interpolate algorithm, the cell types on the background mesh are determined based on their location with respect to the immersed boundary. All the nodes inside the solid boundary are assigned as solid nodes and the rest are assigned as fluid nodes. Moreover, the fluid nodes that lie in the immediate vicinity of the immersed boundary are marked as fluid IB nodes. Figure 2.1 depicts the node types on the background grid.

3. **Boundary treatment**

In this step, modifications are made to the IB node values in order for the fluid nodes to see the presence of the immersed boundary. For each IB node, a probe is assigned which lies on the surface element normal direction and at one cell distance from the IB node. A tri-linear interpolation method is used to determine the value of the desired primitive flow variable at the probe location from the surrounding nodes. The value calculated at the probe is then used in the computation of the value at IB node to satisfy the appropriate boundary condition. The fluid governing equations are solved on the fluid nodes with the IB nodes acting as the de facto boundary with the correct boundary conditions.

4. **Force calculation**

The fluid force is calculated on each surface element of the immersed surface which is defined by an unstructured triangulated mesh. For each surface element, a centroid and normal direction are calculated based on the location of the vertices. Then a probe is assigned that lies along the surface element normal from the element centroid as shown in Figure 2.2. The same tri-linear interpolation method used for IB node probes (but with a different surrounding node stencil) is employed to determine the value of the desired primitive flow variable at the probe location. In the present simulations, pressure and velocity are calculated at the probe location. The distance from the probe to the element \(d_p\) is selected such that no solid node value is used in the interpolation and the
linear gradient assumption is still valid. The force on each element consists of pressure and viscous forces.

**Pressure:**

To estimate the pressure component of the force at each surface element, the non-dimensional material derivative of velocity at the surface is related to the normal pressure gradient as

\[
\frac{d \vec{U}}{dt} = -\frac{1}{\rho} \frac{d P}{d \vec{n}}
\]

by neglecting the viscous contribution to the pressure gradient. By assuming a constant acceleration in the region between the surface element and element probe, Equation 2.5 is discretized as:

\[
a_{\vec{n}} = \frac{(P_p - P_e)}{\rho d_p}
\]

Equation 2.6

Here \(a_{\vec{n}}\) is the surface element acceleration component in the surface normal direction. In the current study, since the particles in assembly are fixed, \(a_{\vec{n}} = 0\). Thus:

\[
P_e = P_p
\]

Equation 2.7

It is to note that in the current formulation, the total pressure is used in calculating the pressure force (mean+fluctuating in Equation 3). This definition is the same as Hill et al. [35] and Tenneti et al. [36], whereas Van Der Hoef et al. [37] and Beetstra et al. [38] define the particle force by subtracting the force component due to mean pressure gradient.

**Shear stress:**

To calculate the viscous forces, the velocity of the fluid at the probe location, \(\vec{U}_p\), is used to calculate the shear stress component at each surface element. The fluid velocity is decomposed into the tangential and surface normal components. In the current study, only the tangential shear stress is used under the assumption that the normal stresses are insignificant. Assuming a linear tangential velocity profile, the non-dimensional shear stress is:
The element surface force is calculated by taking both pressure and shear stress into account:

$$d\vec{F}_e = (\tilde{\tau}_w - P_e \cdot \vec{n})dA$$  \hspace{1cm} \text{Equation 2.9}$$

where $\vec{n}$ is the surface element normal vector.

The fluid force acting on each particle is calculated by integrating the viscous and pressure force on the surface of the particle:

$$\vec{F}_i = \oint_A d\vec{F}_e$$  \hspace{1cm} \text{Equation 2.10}$$

The average drag force on all particles is estimated by:

$$\vec{F}_{g-s} = \frac{1}{N} \sum_{i=1}^{N} \vec{F}_i$$  \hspace{1cm} \text{Equation 2.11}$$

All forces are further normalized using the Stokes-Einstein relation:

$$F = \frac{\vec{F}_{g-s}}{3\pi \mu D_{equ} U}$$  \hspace{1cm} \text{Equation 2.12}$$

2.5 \textbf{Simulation Setup}

2.5.1 \textbf{Geometry, Grid and Simulation Parameters}

In the present study, only a mono-disperse system is considered, i.e. all particles have the same geometric parameters. The computational domain is a cube, with the periodic boundary condition applied along all three directions. A pressure gradient is applied along the x-direction to drive the fluid flow. Particles are randomly distributed in the computational domain, fixed at their initial positions. When the flow reaches a steady state, fluid forces acting on each particle are calculated. By averaging the forces over all the particles in the fluid domain, the drag force is
calculated for a given Reynolds number and solid fraction. Similar methods have already been successfully used to extract drag laws for spherical particles in assembly by Hill et al. [35], Van Der Hoef et al. [37], Beetstra et al. [38] and Tenneti et al. [36].

In all calculations, $U_{ref} = U$, the superficial velocity which equals the x-direction volumetric flowrate divided by the area of the cross-section, and $L_{ref} = D_{eq}$, the equivalent spherical diameter. Thus the Reynolds number is defined as:

$$Re = \frac{\rho UD_{eq}}{\mu}$$  \hspace{1cm} \text{Equation 2.13}$$

where $\rho$ and $\mu$ are the fluid density and dynamic viscosity.

The computational domain is a cube with side $10D_{eq}$. Results from a grid independency study are given in Table 2.1 for ellipsoid particles. Resolutions of 30 to 50 background grid cells per equivalent particle diameter were tested. It is shown that the maximum difference between the three grids is about 2% so 40 grid cells per $D_{eq}$ were deemed to be sufficiently fine to resolve the fluid field around each particle.

Because of the fixed domain size, the number of particles $N$ in the computation domain is a function of solid volume fraction $\phi$ alone:

$$N = \frac{6\phi L^3}{\pi D_{eq}^3} = \frac{6000\phi}{\pi}$$  \hspace{1cm} \text{Equation 2.14}$$

Sphericity $\psi$, proposed by Wadell [39] is the most widely used parameter to quantify the shape of non-spherical particles.

$$\psi = \frac{\frac{1}{\pi^3}(6V_p)^{\frac{2}{3}}}{A_p} = \frac{A_s}{A_p}$$  \hspace{1cm} \text{Equation 2.15}$$

where $A_p$ is the surface area of the particle, $V_p$ is the volume of the particle, and $A_s$ is the surface area of a sphere which has the same volume as the particle. The more spherical a particles is, the closer
this factor gets to one. The geometry parameters and number of particles for each solid fraction are shown in Table 2.2. An ellipsoidal particle shape is chosen because CFD-DEM simulation methods have been developed for such particles[23][40], but the drag correlations used in these studies are not validated. In addition, the drag coefficient for a single isolated ellipsoidal particle as a function of particle orientation and Reynolds number is available in the literature [41]. For 10% solid fraction 191 particles are used which increase to 669 particles for φ=35%. In contrast, past particle resolved simulation studies on assembly of particles have used 32 to 60 particles [35], 54 particles [37][38], 16 to 161 particles [36] for solid fraction between ~0.1 to ~0.5. Tests were conducted to qualify the intended randomness of the particle distribution. Three different random realizations were tested for ellipsoid particles at φ=10% (191 particles), which showed that there was less than 1% difference in the calculated mean drag. The solid fraction for ellipsoids was limited to 35% because beyond this packing density it became difficult to generate a random distribution without particle-particle overlap. To generate distributions with higher solid fractions it would have been necessary to give some preferential orientation to the ellipsoids and would have been outside the scope of this investigation.

2.5.2 Particle assembly

The random particle assembly is generated using a physics simulation engine SDK- PhysX by Nvidia [42]. During the assembly process, each particle is randomly spawned in the designated space and associated with a mesh to represent its geometry. If the particle spawns at a location which has already been occupied by another particle, an overlap is detected between the convex meshes, and the two particles are relocated. This process ensures that a random assembly of particles is created with no overlap. Any shape created by CAD software can be imported and packed in this framework. Figure 2.3 shows packing of: (a) spheres; (b) capsules; (c) cylinders; (d) mixed spheres, capsules,
dodecahedron, cubes, cuboid, cylinders with random size. After the assembly, the location and orientation of each particle is used to create the surface mesh for IBM.

### 2.6 Results - Spherical Particles

To test the current model for calculating drag force, we first simulate randomly packed spherical particles and compare our results with the correlation recently developed by Tenneti et al. [36] who also used particle resolved simulation.

The surface mesh of each sphere is an unstructured mesh consists of about 2000 triangular elements. Six different solid fractions $\phi$, ranging from 0.1 to 0.45, are tested. Reynolds number based on the superficial velocity and diameter are tested at 10, 50, 100 and 200. Drag force on each particle is calculated when the fluid field reaches a steady state.

Figure 2.4 shows the immersed surface identified by GenIDLEST for solid fractions of 10% and 45%. As the solid fraction increases, the interstitial spaces between particles decrease, making it more challenging to accommodate the IBM probes in fluid regions.

Figure 2.5 shows the normalized drag force of spherical particles from the current simulations. The results are compared to the drag correlations developed by Tenneti et al. [36]:

$$F = \frac{F_{iso}(Re)}{(1 - \phi)^3} + F_\phi(\phi) + F_{\phi, Re}(\phi, Re)$$

$$F_\phi(\phi) = \frac{5.81\phi}{(1 - \phi)^3} + \frac{0.48\phi^5}{(1 - \phi)^4}$$  \hspace{1cm} \text{Equation 2.16}$$

$$F_{\phi, Re}(\phi, Re) = \phi^3 Re(0.95 + \frac{0.61\phi^3}{(1 - \phi)^2})$$

where $F_{iso}(Re)$ is the Dalla Valle [43] drag correlation for a single spherical particle.
The current predictions show very good agreement with the correlation when the Reynolds number is less than 200. At Reynolds number of 200, the predicted drag force from the present simulation is 5%~10% higher than the correlation. Tenneti et al. [36] have noted that their predictions, from which the correlation is built, consistently predict a lower drag at Re=200 than that reported by other researchers.

2.7 Results - Ellipsoidal Particles

The simulation setup for calculating the drag force of a random array of ellipsoidal particles is the same as that of spherical particles. The surface grid for each ellipsoidal particle is an unstructured triangular mesh with 2100 cells. Solid fractions $\phi$ of 0.1, 0.2, 0.3 and 0.35 are tested for a Reynolds number ranging from 10 to 200. The number of particles for each solid fraction is shown in Table 2.2. Figure 2.6 shows the immersed surface of ellipsoids at solid fraction of 10% and 35%. Figure 2.7 shows a representative velocity field in the assembly of ellipsoidal particles at Reynolds number of 10 and solid fraction of 0.35. The velocity magnitude is dependent on the local particle packing densities with larger fluid velocities prevailing in regions with small interstitial spaces.

The pressure force and viscous forces, normalized by the Stokes-Einstein relation, are shown in Figure 2.8. The pressure force increases approximately linearly with Reynolds number for both spherical and ellipsoidal particles but the slope is larger for ellipsoids than the slope for spherical particles at the same solid fraction. At the same solid fraction, the difference between ellipsoidal and spherical particles increases as the Reynolds number increases. This trend has also been reported for single isolated particles, the influence of particle shape on drag increases as the Reynolds number increases [9]. At the same Reynolds number, the difference between ellipsoidal and spherical particles increases as the solid fraction increases. The viscous force varies as a sublinear power of the mean flow Reynolds number. The difference in viscous force between ellipsoid and sphere also increases as
the Reynolds number and void fraction increase: at solid fraction of 0.1, the viscous force shows little
difference while at solid fraction of 0.35, the force on the ellipsoids is 15% to 20% larger than
spheres.

In the following section, we compare simulation results to different existing drag correlations
in the literature. The comparison is divided into three categories based on the parameters required by
the correlation: (I) only equivalent spherical diameter ($D_{eq}$) and solid fraction ($\phi$) are used; (II)
particle sphericity $\psi$ is used along with $D_{eq}$ and $\phi$. In these two comparisons, solid fraction is the
only parameter needed from the assembly. (III) The final comparison is at the scale of the particle, in
which each particle’s orientation is used along with $\psi$, $\phi$ and $D_{eq}$ to calculate the drag force. This
method can only be applied to numerical simulations where the detailed orientation of each particle is
available.

2.7.1 Category I: Comparing to spherical particle packing correlations

First we compare IBM results with widely used correlations using the equal volume diameter
as the characteristic length, shown in Figure 2.9. In many two-phase flow research studies with non-
spherical particles, the assumption that the particle shape is spherical is used. This comparison shows
the error introduced by this assumption. The drag force of spherical particle at the same Reynolds
number and solid fraction is also plotted in Figure 2.9. Correlations developed by Wen and Yu[2] and
De Felice[25] have the form of:

$$F(Re, \phi) = F_{iso}(Re)(1 - \phi)^{-\alpha}$$  \hspace{1cm} \text{Equation 2.17}

where $F_{iso}(Re)$ is the drag correlation for isolated single particle, and the neighboring effects are
accounted by the term $(1 - \phi)^{-\alpha}$. $\alpha$ is set to 4.7 in Wen and Yu’s correlation, and $4.7 -
0.65 \exp \left[ -\frac{(1.5 - \log Re)^2}{2} \right]$ in De Felice’s correlation. In the comparisons, the correlation developed by
Turton and Levenspiel [44] and Dalla Valle [43] for single sphere are used for \( F(Re, 0) \). Syamlal and O’Brien [45] developed their drag law based on the terminal velocity correlation from Richardson and Zaki [46]. Finally, Tenneti et al.’s correlation is based on particle resolved simulations.

For all the solid fractions tested in the current work, the drag for ellipsoidal particles is larger than the corresponding force for an assembly of spherical particles from IBM. This force difference increases as the Reynolds number increase. At solid fraction of 0.1, the current simulation results for ellipsoids agree with Syamlal and O’Brien’s correlation and which gives values much larger than other correlations. At solid fraction of 0.2 to 0.35, the Wen and Yu correlation with Dalla Valle exhibits the closest agreement with the current simulation results for ellipsoids while other correlations under-predict by 15% to 50%. We can conclude that no correlations works consistently at all solid fraction range for ellipsoidal particles. It is noteworthy that even for spherical particles, there is considerable deviation between the correlations as Re increases, with the combination of Wen-Yu with Turton and Levenspiel correlations and the correlation of Tenneti et al. giving the best agreement with current results.

2.7.2 Category II: Comparing to non-spherical packing correlations

In this section, we test the performance of combined correlations by substituting the \( F(Re, 0) \) in Wen and Yu (hereinafter referred to as ‘W&Y’) and Di Felice’s correlations with single non-spherical particle drag models. These type of combined correlations have been used in CFD-DEM simulations for predicting drag in non-spherical particle fluidized beds [23][40]. For single non-spherical particles, correlations derived by Harder and Levenspiel (hereinafter referred to as ‘H&L’) [8] and Chien [10] which use the sphericity (\( \psi \)) to describe the particle shape are tested. The drag correlation developed by Bagheri and Bonadonna (hereinafter referred to as ‘B&B’) [16], using the particle flatness, elongation, equivalent diameter and particle-to-fluid density ratio as parameters, is
also tested here. The drag force predicted by the combined correlations and current simulations are plotted in Figure 2.10. For solid fractions of 0.1 and 0.2, all the correlations under-predict the drag force by 5% to 35% for ellipsoids. At solid fraction of 0.3 and 0.35, W&Y with H&L capture the trend while still under predicting by 10% to 27%. W&Y with B&B shows a slight improvement over the W&Y and H&L correlation. However, this combination still under predicts the drag force at low solid fraction. This could be because of the low Reynolds number in this study and the fact that the particle-fluid density ratio term is set to infinity in the correlation because the particles are fixed to their initial positions. Similar to using the spherical particle drag correlation, the non-spherical particle drag correlation when combined with the Di Felice and W&Y correlation, do not give a consistently accurate estimation of drag force for the assembly of ellipsoidal particles.

2.7.3 Category III: Comparing to non-spherical packing correlations with orientation data ($D_{eq}, \psi$ and orientation)

In CFD-DEM studies of packed non-spherical particles, the single non-spherical drag correlation developed by Holzer et al. [13] has been used along with De Felice’s correlation:

$$F(Re, \psi_\parallel, \psi, \psi_\perp) = \left( \frac{8}{Re} \sqrt[3]{\psi_\parallel} + \frac{16}{Re} \sqrt{\psi} + \frac{3}{Re} \psi_\parallel \right) \left( \frac{Re}{24} \right)^{0.42 \times 10^{0.4(-log\psi)^{0.2}}} \left( \frac{1}{\psi_\perp} \right)$$

Equation 2.18

In this equation, $\psi, \psi_\perp$ and $\psi_\parallel$ are the sphericity, crosswise sphericity, and lengthwise sphericity. The crosswise sphericity ($\psi_\perp$) is the ratio between the cross-sectional area of the equal
volume sphere and the projected cross-sectional area of the particle in the flow direction, and the lengthwise sphericity \( (\psi_{\parallel}) \) is the ratio between the cross-sectional area of the equal volume sphere and the difference between half the surface area and the mean projected longitudinal cross-sectional area of the particle. In the current simulations, the orientation of the ellipsoidal particle can be fully described using the angle \( (\alpha) \) which is the angle between the fluid flow direction and the particle’s semi-major axis as shown in Figure 2.11. Each particle’s \( \psi_{\perp} \) and \( \psi_{\parallel} \) can be calculated based on this angle. For the ellipsid particle shape tested in the current study, Zastawny et al. [41] proposed the following correlation for a single isolated particle:

\[
F(Re, \alpha) = F_{\alpha=0} + (F_{\alpha=\pi/2} - F_{\alpha=0}) \sin^2(\alpha)
\]

\[
F_{\alpha=0} = \left( \frac{5.1}{Re^{0.48}} + \frac{15.52}{Re^{1.05}} \right) \left( \frac{Re}{24} \right)
\]

\[
F_{\alpha=\pi/2} = \left( \frac{24.68}{Re^{0.98}} + \frac{3.19}{Re^{0.21}} \right) \left( \frac{Re}{24} \right)
\]

Equation 2.19

(The original drag coefficient correlation is modified based on the normalization by Stoke’s drag used in the present paper.) This correlation is also tested here.

By substituting the above single non-spherical particle correlation into De Felice’s correlation and Tenneti et al.’s correlation, the drag force of each particle in assembly can be estimated. This type of combined correlations have been used in CFD-DEM simulations for predicting drag in non-spherical particle beds [23][24][40].

Figure 2.12 and Figure 2.13 show the normalized drag force on each particle vs the particle orientation \( \alpha \) at solid fraction of 0.1 and 0.35. The scatter markers in the figures are the drag force calculated on each individual particle from one representative simulation at a given solid fraction and Reynolds number. The open squares are averaged force values from the simulation over an interval of \( \pi/36 \). The solid line is the drag force predicted using the combined De Felice and Holzer correlation.
(hereinafter referred to as ‘F&H correlation’), the dash-dot line is the combined Tenneti et al. and Holzer correlation (hereinafter referred to as ‘T&H correlation’), and the dash line is the combined Tenneti et al. and Zastawny correlation (hereinafter referred to as ‘T&Z correlation’). The simulation results show that the particle drag can have significant variance even at the same orientation. However, in general at a given Reynolds number and solid fraction, the mean particle drag tends to increase as the angle $\alpha$ increases.

Using the combined correlations, each particle’s drag force can be calculated based on its orientation, $\alpha$. Table 2.3 shows the normalized mean drag force from the current IBM simulations comparing to F&H, T&H and T&Z correlations. The correlation predictions are based on the orientation data of each individual particle from the simulations. The F&H correlation predicts significantly lower drag force at Reynolds number of 10. At Reynolds number of 50, 100 and 200 and solid fraction of 0.1, the F&H correlation has good agreement with the IBM simulation results. At other solid fractions and Reynolds number, the F&H correlation has 5% to 24% difference with current results. Other than the 15% under prediction at Reynolds number of 10 and solid fraction of 0.35, the T&H correlation agrees very well with the IBM simulation results. The T&Z correlation has relatively good agreement at solid fraction of 0.1 while consistently under predicting the drag value by 9% to 22% at higher solid fractions. Over all, among the three correlations tested here, T&H with 7.15% average difference gives the closest prediction compared to current results, and therefore, should be used for ellipsoidal particles in assembly if the particle shape is similar to the shape studied here.

### 2.8 Summary and Conclusions

In this paper, particle-resolved simulations are performed to study the momentum transfer for nonspherical particles in assembly. A random arrangement of ellipsoidal particles with sphericity ($\psi =$
0.887) is used in the assembly and the particle-fluid boundaries are resolved using the immersed boundary method. The ellipsoidal particles are packed using a physics engine which provides random particle configurations with no overlap between particles. Incompressible Navier-Stokes equations are solved in the fluid with no slip boundary condition applied at the fluid-particle boundary. The fluid field is a periodic cubic domain. The pressure and viscous force on each particle are calculated based on the resolved flow field. Flow through an assembly of spherical particles is tested, and calculated drag forces are compared with previous particle resolved simulation results to validate the current framework. Then packed ellipsoidal particles are simulated in a solid fraction range from 0.1 to 0.35 and at low to moderate Reynolds numbers \((10 \leq Re \leq 200)\). Widely used drag force correlations are evaluated based on the current simulation results.

The following conclusions can be drawn from this study:

- Drag force predicted by current simulations for assembly of spherical particles shows good agreement with previous study. The framework developed in this study is reliable to investigate the drag force for assemblies of non-spherical particles.

- Drag force of ellipsoidal particle assemblies is 15% to 35% larger than equal volume spherical particles at the same solid fraction and Reynolds number.

- The performance of available drag correlations applied to non-spherical particles is examined. Correlations based only on particle equal volume sphere diameter \(D_{eq}\) under predict the drag force. Combined correlations using particle shape factors and particle equal volume sphere diameter \(D_{eq}\) also under predict the drag force: the correlations give 2% to 35% smaller drag forces than the current particle resolved simulation results.
Combined correlations taking the particle orientation into account show better agreement. The combined Tenneti et al. and Holzer correlation, with 7.15% average error, has the closest prediction capability with current simulation results.

2.9 Acknowledgements

Danesh Tafti would like to acknowledge support from the National Energy Technology Laboratory (NETL) as ORISE Faculty. The authors acknowledge Advanced Research Computing at Virginia Tech for providing computational resources and technical support that have contributed to the results reported within this paper. URL: http://www.arc.vt.edu.
2.10 Nomenclature

\[ A \] area
\[ d \] distance
\[ D_{eq} \] equal volume sphere diameter
\[ F \] normalized force
\[ L \] length
\[ N \] number of particles
\[ n \] surface normal
\[ \mathbb{P} \] pressure
\[ \mathbb{R} \] Reynolds number
\[ t \] time
\[ u \] streamwise interstitial velocity
\[ U \] superficial flow velocity

Greek

\[ \alpha \] angle describing ellipsoidal particle orientation
\[ \beta \] mean pressure gradient constant
\[ \rho \] density
\[ \mu \] viscosity
\[ \phi \] solid fraction
\[ \psi \] sphericity
\[ \tau \] shear stress

Subscripts
$e$  surface element

$p$  probe

Superscripts

*  dimensional value

Miscellaneous

$x, y, z$  Cartesian coordinates
### 2.11 Tables

Table 2.1. Grid independence study for packed ellipsoidal particles at solid fraction of 0.1

<table>
<thead>
<tr>
<th>Re</th>
<th>F 30 cells per $D_{eq}$</th>
<th>F 40 cells per $D_{eq}$</th>
<th>F 50 cells per $D_{eq}$</th>
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Table 2.2. Geometry parameters and the number of particles for each solid fraction.

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<th>Ellipsoid Semi-major 0.921</th>
<th>Semi-minor 0.368</th>
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<tr>
<td>Sphericity $\psi$</td>
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<td></td>
</tr>
<tr>
<td>$D_{eq}$</td>
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<td>1</td>
<td></td>
</tr>
<tr>
<td>Number of particles ($N$)</td>
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<td></td>
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</tr>
<tr>
<td>$\phi = 10%$</td>
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<td>191</td>
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<tr>
<td>$\phi = 20%$</td>
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<td>$\phi = 45%$</td>
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Table 2.3. Normalized mean drag force from current simulation compare to F&H, T&H and T&Z correlation.

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<th>IBM</th>
<th>F&amp;H</th>
<th>% diff</th>
<th>T&amp;H</th>
<th>% diff</th>
<th>T&amp;Z</th>
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2.12 Figures

Figure 2.1. Node type on the background fluid mesh
Figure 2.2. Pressure and Shear stress calculation
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Figure 2.4. Immersed surface of spherical particles at : (1) solid fraction of 10%; (2) solid fraction of 45%
Figure 2.5. Normalized drag force from IBM compared to drag correlation developed by Tenneti et al. [36] using particle resolved simulations.
Figure 2.6. Immersed surfaces of ellipsoidal particles at (1) 10% solid fraction (2) 35% solid fraction.
Figure 2.7. Representative velocity field (fluid flow in x-direction) at Reynolds number of 10 and solid fraction of 0.35.
Figure 2.8. Normalized pressure force and viscous force.
Figure 2.9. Normalized drag force of spherical and ellipsoidal particles compared to widely used correlations for spherical particles in assembly.
Figure 2.10. Normalized drag force of ellipsoidal particles comparing to modified correlations.
Figure 2.11. Particle orientation
Figure 2.12. Normalized drag force on each particle vs the particle orientation $\alpha$ at solid fraction of 0.1.
Figure 2.13. Normalized drag force on each particle vs the particle orientation $\alpha$ at solid fraction of 0.35.
Chapter 3
Heat Transfer in an Assembly of Ellipsoidal Particles at Low to Moderate Reynolds Numbers

3.1 Abstract

Fixed and dynamic assemblies of non-spherical particles participate in many heat and mass transfer industrial processes. However, most convective heat transfer coefficients are adapted from correlations available for spherical particles by using the concept of equal volume spheres or in some cases the sphericity, which is a measure of deviation from a spherical shape. In this study, Particle-Resolved Simulations (PRS) are performed to investigate the heat transfer in flow through a fixed random assembly of spherical and ellipsoidal particles of aspect ratio 2.5:1. The assembly of particles is simulated for solid fractions between 0.1 to 0.35 using 191 to 669 particles, respectively, at low to moderate Reynolds numbers ($10 \leq Re \leq 200$). The random particle assembly is generated using a physics simulation engine SDK- PhysX. The particle-fluid boundaries are resolved using the Immersed Boundary Method (IBM) with a constant heat flux boundary condition. Simulation results in the ellipsoidal assembly show that the local velocity and temperature field are significantly affected by the particle orientation. Mean Nusselt numbers for the ellipsoidal assembly are consistently larger than spherical particles when Reynolds number is more than 10, and the difference increases as the Reynolds number increases. A Nusselt number correlation is proposed based on the simulation data. The proposed correlation is valid in the
range $10 \leq Re \leq 50$ for solid fraction of $0 < \phi \leq 0.35$, and $50 < Re \leq 200$ for solid fraction of $0.1 \leq \phi \leq 0.35$.

### 3.2 Introduction

Fluid-particulate mixtures participate in many heat and mass transfer industrial processes such as petroleum refining, blast furnaces, solid fuel combustion and gasification, chemical looping, CO2 capture, drying of powders, etc. Thus extensive experimental and numerical studies have been devoted to understanding the interphase momentum and heat transfer in such flows during the last several decades. Particle drag coefficient and Nusselt number behavior in assembly are two important parameters in interphase transfer terms. A number of correlations have been developed, for example, the Wen and Yu [47] correlation and Ergun [3] correlation for predicting drag, and Gunn [48] correlation and Wakao and Kaguei[49] correlation for predicting heat transfer in fluid-particle mixtures. However, to simplify the problem, most of these studies and correlations assume spherical particles, which are rarely present in most natural and industrial processes. Non-spherical particles not only add complexity to the particle-particle packing structure, but also strongly affect the velocity and temperature field of the fluid by influencing the momentum and heat transfer between the fluid and solid phase. For example, a recent particle-resolved simulation (PRS) study showed that at the same solid fraction and Reynolds number, the average drag coefficient of ellipsoidal particles in random assemblies is 15% to 35% larger than equivalent spherical particles [50]. Similar large discrepancies are expected to exist when spherical
Particle heat transfer correlations are applied to non-spherical particles. Thus it is imperative that careful studies be conducted to evaluate the current state-of-the-art because these correlations are routinely used for calculating convection heat transfer in methods in which the particles are treated as point masses.

Past heat transfer correlations for fluid-particulate systems have mostly relied on experimental data. Gunn [48] first developed a theoretical equation which yields to a constant Nusselt number at low Reynolds number based on a stochastic model of particle-particle void space. By including this equation as an asymptotic condition, a Nusselt number correlation, shown in Equation (1), was proposed to fit experimental data from many sources. This correlation can give an estimate of Nusselt number within the porosity range of 0.35 to 1.0 and Reynolds number up to $1 \times 10^5$.

$$Nu = (7 - 10\epsilon + 5\epsilon^2)\left(1 + 0.7Re^{0.2}Pr^{1/3}\right) + (1.33 - 2.4\epsilon + 1.2\epsilon^2)Re^{0.7}Pr^{1/3}$$

Equation 3.1

Although this correlation is widely used, it is noted that the experimental data used for constructing this correlation had large scatter over several orders of magnitude [49,51].

Wakao et al. [49] collected experimental data of heat transfer coefficients from 27 published literature sources. After a critical review of the accuracy of these data, the following correlation was proposed:

$$Nu = 2 + 1.1Pr^{1.3}Re^{0.6}$$

Equation 3.2

This correlation assumes a densely packed bed and hence void fraction dependence is not taken into consideration. Therefore, this correlation is not valid for an assembly of particles.
Because of the abrasive and opaque environment encountered in fluid-particle systems, experimental measurements of detailed velocity and temperature fields are quite challenging. While mean heat transfer coefficients in packed beds can be experimentally measured by energy balances, to measure heat transfer coefficients at lower solid fractions for suspended particles in assembly is quite challenging. Additionally, experimental approaches would find it very difficult to resolve interstitial velocity and temperature fields for detailed characterization. Thus, several computational approaches have been developed to aid the fundamental understanding of inter-phase interactions. Amongst these approaches, particle resolved simulations [35,37,52–55] with their ability to resolve the flow and temperature field in the interstitial spaces between particles in assembly can directly calculate the heat transfer by individual particles. Deen et al. [56] developed a particle resolved simulation technique in which they used the immersed boundary method to resolve the particle fluid boundary while employing discrete particle approach with hard sphere model for particle-particle and particle-wall collision. They studied the momentum and heat transfer in stationary arrays of spherical particles and in a fluidized bed. Tenneti et al. [53] studied the heat transfer in steady flow past statistically homogeneous random assemblies of stationary spherical particles using a 3D particle resolved simulation. In their research, a thermal similarity boundary condition is imposed on the temperature field by drawing analogy from thermally fully developed flow in pipes. The particles in the assembly are fixed at the initial positions and held at constant uniform temperature. Based on Tenneti’s work, Sun et al. [51] studied fluid-particle heat transfer in packed spherical particles with slip Reynolds number from 1 to 100 and solid fractions from 0.1 to 0.5, and a new Nusselt number correlation was
proposed to fit the simulation data. Tavassoli [57] studied the heat transfer coefficient (HTC) of bi-disperse random array of spheres with a size ratio of 1:2. They found that for the bi-disperse sphere system they tested, the correlation of the monodisperse HTC can estimate the average HTC well if the Reynolds and Nusselt numbers are based on the Sauter mean diameter. Compared to the many studies of assembly of spherical particles, only few studies of heat transfer in assemblies of non-spherical particle have been reported. Yang et al. [58] studied flow in ordered packed spheres and ellipsoid particles and found that the pressure drop and heat transfer performance is greatly affected by the packing structure and the particle shape. Tavassoli et al. [59] studied heat transfer in a random assembly of spherocylinders using particle resolved simulations. In their study, the total number of simulated particles are fixed at 30, and the variation in solid volume fraction is achieved by changing the size of the fluid domain. They proposed that the heat-transfer correlation for spherical particles can be used for spherocylinders if a proper characteristic diameter is chosen. Besides these few studies focusing on assemblies of non-spherical particles, there are several heat transfer studies for isolated non-spherical particles: long cylinders [60], ellipsoid [61], elliptic cylinder [62], spheroid [63,64] and cubic particle [65,66].

The objective of this study is to use Particle-Resolved Simulations (PRS) to investigate the heat transfer through a fixed random assembly of spherical and ellipsoidal particles of major to minor axis ratio of 2.5 in the range of \( 10 \leq Re \leq 200 \) and \( 0.1 \leq \phi \leq 0.35 \). The random particle assembly, with 191 to 669 particles based on the solid fraction, is generated using a physics simulation engine SDK- PhysX. The particle-fluid boundaries are resolved using the Immersed Boundary Method (IBM) with constant heat flux boundary
conditions. For each solid fraction and Reynolds number, simulation results are averaged based on three different random configurations to have an adequate sample size.

The paper presents the governing equations and the major components of the IBM method. The model is first used to simulate an assembly of spherical particles. Average Nusselt numbers for spherical particles are compared with widely used heat transfer correlations and particle resolved simulation data from past studies. A similar model is then applied to the assembly of ellipsoidal particles and differences with spherical particles are highlighted. Finally, a Nusselt number correlation for the ellipsoidal particle geometry tested is proposed.

### 3.3 Governing Equations and Methodology

All simulations are performed using an in-house code – Generalized Incompressible Direct and Large Eddy Simulation of Turbulence (GenIDLEST). The details of the framework and methodology used in GenIDLEST can be found in Tafti [31] and Tafti [67]. In this section, the relevant governing equations are presented along with some details of the Immersed Boundary Method [28]. GenIDLEST with immersed boundary method has already been successfully applied to oscillating cylinders [28], turbine cooling passage heat transfer [29], fluid structure interactions problems [30] and momentum transfer in fluid-particle system [50].

#### 3.3.1 Governing Equation and Numerical Method

The non-dimensional form of the Navier-Stokes equations under the incompressible assumption are as follows:
Continuity:
\[
\frac{\partial u_i}{\partial x_i} = 0 \quad \text{Equation 3.3}
\]

Momentum:
\[
\frac{\partial u_i}{\partial t} + \frac{\partial (u_j u_i)}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j} \left\{ \frac{1}{Re_{ref}} \left( \frac{\partial u_i}{\partial x_j} \right) \right\} \quad \text{Equation 3.4}
\]

Energy:
\[
\frac{\partial T}{\partial t} + \frac{\partial (u_j T)}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \frac{1}{Re_{ref} Pr_{ref}} \frac{\partial T}{\partial x_j} \right) \quad \text{Equation 3.5}
\]

where the non-dimensionalizations are:
\[
x_i = \frac{x_i^*}{L_{ref}}, \quad u_i = \frac{u_i^*}{u_{ref}^*}, \quad t = \frac{t^* u_{ref}^*}{L_{ref}^*}, \quad P = \frac{p^* - P_{ref}^*}{\rho_{ref}^* u_{ref}^*}, \quad Re_{ref} = \frac{\rho_{ref}^* u_{ref}^* L_{ref}^*}{\mu_{ref}^*}, \quad T = \frac{T^* - T_{ref}^*}{T_o^*}, \quad Pr_{ref} = \frac{C_p \mu_{ref}^*}{k_{ref}^*}
\]

The above governing equations are transformed to generalized coordinates, and discretized in a conservative finite-volume formulation using a second-order central (SOC) difference scheme on a non-staggered grid topology. Cartesian velocities, pressure and temperature are calculated and stored at the cell center, whereas fluxes are calculated and stored at cell faces. A projection method using second order predictor-corrector steps is used for the time integration of the continuity and momentum equations. In the predictor step, an intermediate velocity field is calculated; and in the corrector step, an updated divergence free velocity is calculated at the new time-step by solving a pressure-Poisson equation. The pressure-Poisson equation is solved for the cell face fluxes to emulate a staggered grid arrangement. The Biconjugate gradient stabilized method (BiCGSTAB) with a domain-decomposed additive Schwarz Jacobi preconditioner is used to solve the pressure-Poisson equation.
3.3.2 **Immersed boundary method**

The immersed boundary method (IBM) used in this paper is an indirect forcing sharp interface approach. This method is an extension of a scheme originally proposed by Gilmanov and Sotiropoulos [34], and has been modified to fit the generalized coordinate system and non-staggered grid framework of GenIDLEST. In this method, the governing equations are solved without modification for the computational grid in the fluid domain. Special treatment is only applied to the first layer of the fluid nodes (fluid IB nodes) next to the immersed boundary. The major steps of this method are summarized below. The details can be found in Nagendra et al. [28].

5. **Definition of surface grid**

The immersed boundary is the fluid/solid interface which is provided as input in a discretized form of an unstructured triangulated surface mesh. Each of the immersed boundary elements has information of surface normal, area, and location with respect to the fixed background fluid mesh.

6. **Node identification**

By employing a search-locate and interpolate algorithm, the cell types on the background mesh are determined based on their location with respect to the immersed boundary. All the nodes inside the solid boundary are assigned as solid nodes and the rest are assigned as fluid nodes. Moreover, the fluid nodes that lie in the immediate vicinity of the immersed boundary are marked as fluid IB nodes. Figure 3.1. Node type on the background fluid mesh depicts the node types on the background grid.

7. **Boundary treatment**
In this step, modifications are made to the IB node values in order for the fluid nodes to sense the presence of the immersed boundary. With the aim of preserving second order accuracy, for each IB node, two probes are assigned which lie on the surface element normal direction and at one and two cell distance from the IB node, $P_1$ and $P_2$, respectively, in Figure 3.2(a). A second order interpolation method is used to determine the value of the desired primitive flow variable at the probe location ($\psi_{p1}$ and $\psi_{p2}$) from the surrounding background nodes. Second-order accuracy is achieved by using Taylor expansions for $\phi_{ib}$, $\phi_{p1}$ and $\phi_{p2}$ defined about the value at the IB surface $\psi|_{bc}$ - eliminating $\psi|_{bc}$ and $\frac{\partial^2 \psi}{\partial n^2}|_{bc}$ for Dirichlet condition, or $\frac{\partial \psi}{\partial n}|_{bc}$ and $\frac{\partial^2 \psi}{\partial n^2}|_{bc}$ for Neumann condition. The $\psi_{ib}$ can be obtained by the following expressions:

**Dirichlet condition:**

$$\psi_{ib} = \frac{(d_{ib} - d_{p2})d_{ib}d_{p2}\psi_{p1} + (d_{p1} - d_{ib})d_{ib}d_{p1}\psi_{p2} + (d_{ib} - d_{p1})(d_{ib} - d_{p2})(d_{p1} - d_{p2})\psi}{(d_{p1} - d_{p2})d_{p1}d_{p2}}$$

**Equation 3.6**

**Neumann condition:**

$$\psi_{ib} = \frac{(d_{ib}^2 - d_{p2}^2)\psi_{p1} + (d_{p1}^2 - d_{ib}^2)\psi_{p2} - (d_{ib} - d_{p1})(d_{ib} - d_{p2})(d_{p1} - d_{p2})\frac{\partial \psi}{\partial n}|_b}{d_{p1}^2 - d_{p2}^2}$$

**Equation 3.7**

The fluid governing equations are then solved on the fluid nodes with the IB nodes acting as the de facto boundary with the correct boundary conditions. Equation 3.6 and Equation 3.7 are used to find the effective IB node value of velocity, pressure and temperature with the
imposition of the Dirichlet condition for velocity (Equation 3.6) and the Neumann condition (Equation 3.7) for pressure and temperature.

8. **Post-processing**

Several properties at the immersed surface, for example, temperature are calculated in the post-processing step. Similar to the method used for calculating the IB node value, two probes are placed in the surface element normal direction at one and two cell distance from the surface element centroid, $P_1$ and $P_2$, respectively, in Figure 3.2(b). As before, Taylor expansions are formulated for $\psi_{p1}$ and $\psi_{p2}$ based on $\psi|_{bc}$. When a Neumann condition is applied at the boundary, for example, the constant heat flux boundary condition, the temperature at the immersed surface can be obtained by the following expression:

$$
\psi|_{IS} = \frac{(d_{p2} - d_{p1})d_{p1}d_{p2}\frac{\partial\psi}{\partial n}|_{bc} - d_{p2}^2\psi_{p1} + d_{p1}^2\psi_{p2}}{d_{p1}^2 - d_{p2}^2} \tag{Equation 3.8}
$$

**3.4 Computational Details**

3.4.1 **Geometry, Boundary Conditions and Simulation Parameters**

The computational geometry used for the simulations is shown in Figure 3.3. The X-direction which is also the flow direction extends from -10 to $15D_{eq}$, where $D_{eq}$ is the equivalent sphere diameter of each particle. The particle assembly is placed between $X = -5D_{eq}$ and $5D_{eq}$, with buffer regions upstream and downstream of this section as shown in the
Figure. The cross-stream, Y- and Z- directions both extend 10 $D_{eq}$. The particles are randomly distributed in the assembly region and fixed at their initial positions.

Flow enters the domain at X= -10 $D_{eq}$ with a velocity $u_x=U_{in}$ and exits at X=15 $D_{eq}$. A zero gradient condition for velocity and temperature is used at the exit to the domain. Cross-stream Y- and Z- directions are assumed to be periodic. By allowing solid particles to be cut at periodic boundaries, true periodicity is imposed for both the solid particles as well as the fluid field. To study the heat transfer, a constant heat flux boundary condition is applied at each particle surface. Constant temperature boundary conditions at low flow rates (low Reynolds number) and high solid fractions posed numerical difficulties because the flow quickly saturated to the particle temperature resulting in unphysically large heat transfer coefficients. In all calculations, $U_{ref} = U_{in}$, the superficial velocity which equals the X-direction volumetric flowrate divided by the area of the cross-section, and $L_{ref}^* = D_{eq}$, the equivalent spherical diameter. The reference temperature $T_{ref}^* = T_{in}$, the inlet flow temperature, and $T_0^* = q''_s D_{eq} / k_{ref}^*$, where $q''_s$ is the specified heat flux on the surface of each particle. Thus the Reynolds number is defined as:

$$Re = \frac{\rho U_{in} D_{eq}}{\mu}$$  \hspace{1cm} \text{Equation 3.9}

where $\rho$ and $\mu$ are the fluid density and dynamic viscosity. All the fluid physical properties are assumed to be constant.

In the present study, only a mono-disperse system is considered, i.e. all particles have the same shape parameters. Because of the fixed domain size, the number of particles $N$ in the computation domain is a function of the solid volume fraction $\phi$ alone:
\[ N = \frac{6\phi L^3}{\pi D_{eq}^3} = \frac{6000\phi}{\pi} \]  

**Equation 3.10**

The particle shape parameters and the number of particles for each solid fraction are shown in **Table 3.1**. The solid fraction for ellipsoids was limited to 35% because beyond this packing density it became difficult to generate a random distribution without particle-particle overlap. To generate distributions with higher solid fractions it would have been necessary to give some preferential orientation to the ellipsoids and would have fallen outside the scope of this investigation in which our primary interest is random assemblies.

The random particle assembly is generated using a physics simulation engine SDK-PhysX by Nvidia [42]. During the assembly process, each particle is randomly spawned in the designated space and associated with a surface mesh to represent its geometry. If the particle spawns at a location which has already been occupied by another particle, an overlap is detected between the meshes, and the two particles are relocated. This physics engine ensures that a random assembly of particles is created with no overlap between particles. More details about the method of assembly can be found in [50]. After the assembly, the location and orientation of each particle is used to create the surface mesh. Figure 3.4(a) shows one packing configuration of ellipsoid particles at solid fraction of 20%. The immersed surface of each particle is represented by an unstructured mesh which contains 2172 triangle elements, which is shown in Figure 3.4(b).
3.4.2 Nusselt number

In the present study, a constant heat flux boundary condition is applied at all particle surfaces. Fluid enters the domain at a low temperature, is heated by the particles, and exits the domain at a higher temperature. Because periodic boundary condition are set in Y and Z direction, the heat transfer problem is only statistically inhomogeneous in the mean flow direction (along X-axis) and all quantities are averaged over the Y-Z plane. The heat transfer coefficient is defined as:

\[
h(x) = \frac{q_s''}{\overline{T_s(x)} - \overline{T_m(x)}}\]

Equation 3.11

where \(q_s''\) is the constant heat flux at the particle surface. \(\overline{T_s(x)}\) is the average temperature at the immersed surface at a given X-location, and \(\overline{T_m(x)}\) is the average mixed mean temperature at the same X-location in the assembly. In non-dimensional terms, Eqn. (11) can be written as

\[
Nu(x) = \frac{1.0}{\overline{T_s(x)} - \overline{T_m(x)}}\]

Equation 3.12

Note that \(\overline{T_s(x)}\) and \(\overline{T_m(x)}\) are obtained over multiple particles by averaging in the Y-Z plane at each X-location.

\[
\overline{T_s(x)} = \frac{1}{\Omega} \int_{\Omega} T_s(x) \, dl
\]

Equation 3.13

\(\Omega\) is the perimeter of the immersed surface cut by the Y-Z plane at a given X-location. \(T_s\) is the local temperature at the immersed surface. The “mixed mean” temperature at each X location is defined as:
\[
\bar{T}_m(x) = \frac{\int_{A_f} |u_x|T \, dA}{\int_{A_f} |u_x| \, dA}
\]

Equation 3.14

where \( u_x \) is the interstitial fluid velocity in the x direction; \( A_f \) is the area occupied by the fluid phase. The mean Nusselt number (\( Nu \)) for the assembly is calculated by averaging \( Nu(x) \) over the interval -3\( D_{eq} \leq X \leq 3\( D_{eq} \) to avoid flow and thermal entrance and exit effects from the particle assembly. Also calculated and reported is the standard deviation (SD) of fluctuating \( Nu(x) \) about the mean value, \( Nu \).

3.4.3 Grid Independency

A grid independency study was conducted in a smaller computation domain of size 25\( D_{eq} \times 5D_{eq} \times 5D_{eq} \) with the same boundary conditions. Computational grids of 30, 40, and 50 background grid cells per equivalent spherical diameter for resolving the particle assembly were investigated. The mean Nusselt number for the assembly and the standard deviation calculated at different resolutions is given in Table 3.2. The maximum difference between the three grids is about 2% in the mean value and 4% in the standard deviation.

Given the relative insensitivity of the mean Nusselt number and its standard deviation to the background grid in the range of 30 to 50 cells per equivalent diameter, 40 grid cells per \( D_{eq} \) were deemed to be sufficiently fine to resolve the fluid and temperature field around each particle. The total number of cells is 560 \( \times \) 400 \( \times \) 400 in the X, Y and Z directions, respectively, for a total cell count of 89.6 million. The calculations are run on 100 processing cores and a typical calculation takes 30 wall clock hours to converge to the final solution.
3.5 Results and discussion

3.5.1 Spherical particles

To validate our methodology for calculating Nusselt number, we first simulate randomly packed spherical particles and compare our results with the correlation developed by Gunn [48], Tavassoli [55] and Sun et al. [51]. The surface mesh of each sphere is an unstructured mesh consisting of about 2000 triangular elements. Four different solid fractions $\phi$, ranging from 0.1 to 0.35 are tested. For each solid fraction, three different random packing configurations are tested. Reynolds number based on the superficial velocity and diameter are tested at 10, 50, 100 and 200. Prandtl number is set at 0.74. The Nusselt number of each simulation is calculated when the fluid field reaches a steady state.

Figure 3.5(a) shows the immersed surface identified by GenIDLEST for an assembly with solid fraction of 20%. Figure 3.5(b) shows the non-dimensional u-velocity on X-Y plane at $Z = 0$ when the Reynolds number is 200. The flow has a uniform u-velocity before entering the particle assembly region, which starts to accelerate due to the blockage of the particles and gets non-uniform with velocity varying from -0.5 to 2.5. Recirculating regions exist in the wake of particles. After exiting the packed region, the variation in u-velocity decrease as the flow moves towards the outlet. Figure 3.5(c) shows the non-dimensional temperature at the same plane. Because a positive constant heat flux boundary condition is applied at the immersed surface, fluid temperature increases as it flows through the packed region. When a particle lies in the wake of another particle, the low velocity in the wake will reduce the effective interstitial Reynolds number and the heat transfer coefficient on the
particle. This in turn will lead to a higher particle surface temperature. This phenomenon has been observed in past studies on inline spheres [68]. Figure 3.5(d) and 5(e) show the non-dimensional u-velocity and temperature at the mid plane of the packed region ($X = 0$) where a strong correlation exists between regions of accelerated flow and low temperatures and vice versa, alternately yielding high and low heat transfer coefficients, respectively. Figure 3.6 shows the temperature at the particle surfaces using Equation (8) for solid fraction of 20% at Reynolds number of 200. In general, the temperature at the immersed surface increases in the flow direction as the temperature of the fluid surrounding the particle increases. On most particles, the windward side exhibits lower surface temperatures because of flow impingement and higher heat transfer coefficients, whereas the downwind or wake side exhibit higher surface temperatures.

Figure 3.7(a) shows the average temperature at the particle surface $\bar{T}_s$ (calculated using Equation 13) and mixed mean temperature $\bar{T}_m$ (calculated using Equation 14) vs X. The mixed mean temperature $\bar{T}_m$ remains at zero before entering the particle assembly and starts to increase at a nearly constant rate in the particle assembly, leaving the assembly at a constant temperature of 0.085. This agrees well with the temperature field shown in Figure 3.5(c). The particle surface temperature $\bar{T}_s$ increases along with $\bar{T}_m$ but exhibits fluctuations about a linear increase. This is due to the non-uniformity of the velocity field in the vicinity of each particle and its effect on the heat transfer coefficient and the surface temperature. These fluctuations are accentuated at the entrance and exit of the particle assembly because of the abrupt change in the flow and thermal fields. Figure 3.7(b) shows the calculated Nusselt number vs X. The entrance and exit effects are also observed here. Because of these
fluctuations, which are not representative of the interior of the assembly, the mean Nusselt number and its standard deviation (SD) is only calculated from $X = -3$ to $X = 3$ in all cases.

Three different random packing configurations are tested for each solid fraction. The mean Nusselt number and standard deviation (SD) for each solid fraction are calculated by gathering the Nusselt number data from all three configurations. In Figure 3.8, current simulation results are compared with the correlations developed by Gunn [48], Tavassoli [55], Sun et al. [51] as well as their raw simulation results from which the correlations were developed (there is no simulation data available in the references at $\phi = 0.35$). The Gunn correlation is developed based on multiple experimental data with an asymptotic condition for low Reynolds number. Although this correlation is widely used, it should be noted that the experimental data used for developing this correlation has considerable scatter over several orders of magnitude [49] [51]. Correlations developed by Tavassoli and Sun et al. are based on particle resolved simulation data. Tavassoli’s simulations had a total of 54 particles, and the domain size was varied to simulate different solid void fractions. Because of this, it would have been difficult to distinguish between the thermally developing and fully-developed regions in calculating the Nusselt numbers, particularly as the solid fraction increased and the domain shrank in size. Sun et al. assumed periodicity in the streamwise direction, thus assuming fully-developed flow and thermal conditions. As one can see, these correlations behave quite differently from each other. The correlation developed by Sun et al. has a similar Reynold number dependence as Gunn’s correlation, however Sun et al.’s correlation shows values 15% to 30% smaller than Gunn’s correlation. Tavassoli’s correlation agrees well with Sun et al.’s correlation at Reynolds number of 10 at all solid
fractions, while the dependence on Reynolds number does not agree with Gunn and Sun et al.’s correlations. It should also be noted that a constant temperature boundary condition is applied at the particle surface in Sun et al and Tavassoli’s simulations. While because Gunn’s correlation is developed from fitting experimental data points with an asymptotic theoretical condition, it is not clear what thermal boundary condition is used on the particle surface for calculating the Nusselt number. In current simulation, a constant heat flux boundary condition is applied at the particle surface.

Our present results show good agreement with Sun et al.’s simulation data. Most of the data points from Sun et al.’s simulation lie within one standard deviation of the current results. Comparing to Sun et al.’s correlation, the current predictions agree well at solid fractions 0.1 and 0.2, while showing a different Reynolds number dependence at solid fractions of 0.3 and 0.35. This is probably because there is no data point available at higher Reynolds number, leaving the fitted function of Sun et al.’s correlation overly influenced by their data at Reynolds number ≤ 100. It is noteworthy that at solid fraction 30%, the trend in Sun et al.’s data is different from what their correlation suggests. The current predictions agree reasonably well with Sun et al.’s data points at solid fraction of 30%, while having a different trend than their correlation. As the Reynolds number increases, the Nusselt number in Tavassoli’s correlation increases faster than other correlations. This could be because of the longer thermal development length at higher Reynolds numbers and the inclusion of this region in their Nusselt number calculation [51].
3.5.2 Ellipsoidal particles

Similar to the spherical particles, an assembly of ellipsoidal particles are simulated at Reynolds number of 10, 50, 100 and 200, at solid fractions of 0.1, 0.2, 0.3 and 0.35. The geometrical parameters and number of ellipsoidal particles packed in each solid fraction are shown in Table 3.1. A constant heat flux boundary condition is applied at the ellipsoidal particle surface, and the Prandtl number is set at 0.74.

Figure 3.9(a) shows the immersed surface identified by GenIDLEST for the ellipsoidal particle assembly at a solid fraction of 20%. Figure 9(b) shows the non-dimensional u-velocity on X-Y plane at Z = 0 for a Reynolds number of 200. The velocity field is highly disturbed due to the presence of the ellipsoid particles with the velocity varying from -0.5 to 2.5. Compared to the velocity contours in Figure 3.5(b) for spheres, the velocity in the ellipsoidal particle assembly is more non-uniform than in the spherical particle assembly because the flow field near an ellipsoidal particle is not only affected by the location of nearby particles but also by the orientation of these particles. Figure 3.9(c) shows the non-dimensional temperature field on the same plane. The thermal wakes of particles with their minor axis aligned with the flow direction are much more prominent than when the major axis is aligned with the flow direction. The correlation between accelerated interstitial flow velocities and lower temperatures and thinner thermal boundaries is evident in Figure 3.9(d) and (e) which plot the u-velocity and temperature at the mid plane of the packed region (X = 0). Figure 3.10 shows the temperature at the immersed surface of the ellipsoidal particles at Reynolds number of 200 and solid fraction of 0.2. In general, temperature at the immersed surface increases as the fluid flows through the assembly. Due to the relatively higher flow
velocity on the windward side, the windward side has higher heat convection than the downwind side, leaving a lower surface temperature at the front side than the back side. Figure 3.10 (c) shows a partial enlarged look at the non-uniform temperature on the particle surface.

Using the same method as used for the spherical particle assembly, the Y-Z plane averaged surface temperature and mixed mean temperature are shown in Figure 3.11(a). The mixed-mean temperature in the ellipsoidal particle assembly is higher than that for spherical particles. This is because the ellipsoidal particle has a larger surface area than the equivalent spherical particle and more thermal energy is transferred to the fluid. Interestingly, the surface temperature of the ellipsoidal particles is much lower than that observed for spherical particles, pointing to a higher heat transfer coefficient. Figure 3.11(b) shows the Nusselt number distribution in X which suggests that the mean Nusselt number is about 30-40% higher than the equivalent spherical assembly.

Similar to the spherical particles, the mean Nusselt number and standard deviation (SD) for ellipsoidal particles at each solid fraction and Reynolds number are calculated by gathering the Nusselt number data from three random configurations while excluding the entrance and exit effects. Figure 3.12 shows the comparisons of the mean and standard deviation from three different random configurations at solid fractions of 0.1 and 0.35. It is observed that the relative variation of Nusselt number about its mean value is higher at $\phi = 0.1$ than at $\phi = 0.35$. This is because of less number of particles in the assembly and as a consequence the thermal field surrounding individual particles could vary substantially from one particle to the other, thus yielding a larger variation in the Nusselt number. Conversely,
at higher fractions the larger number of particles lends some measure of uniformity to the thermal field surrounding each particle and thus results in smaller variation in the Nusselt number. Another trend that is observed is that there is a relative increase in the standard deviation as the Reynolds number increases for both solid fractions. This can be explained by observing that at lower Reynolds numbers the thermal field is dominated by a high thermal diffusivity which yields larger thermal influence zones around each particle and reduces the variability in the thermal field surrounding each particle. Whereas, as the Reynolds number increases, thermal convection starts dominating decreasing the uniformity of the thermal field which now shows a larger dependency on the arrangement of particles. It is also noteworthy that the variation in the mean Nusselt number between different random arrangements, falls well within the standard deviations calculated for individual runs, validating that the results are statistically converged.

Figure 3.13 shows the mean value of Nusselt number vs solid fraction for different Reynolds numbers. In general, at the same Reynolds number, the Nusselt number increases as the solid fraction increases. This is because of greater flow acceleration in the interstitial spaces between particles which increases the local flow Reynolds number. A similar trend is also reported by Sun et al. [51]. At Reynolds number of 10, the difference in Nusselt number between ellipsoidal particles and spherical particles is not significant because of the predominance of thermal diffusivity effects which mask the actual shape of the particle. At Reynolds numbers higher than 10, the Nusselt numbers for ellipsoidal particles are consistently higher than spherical particles. Richter and Nikrityuk [61] observed a similar trend for an isolated ellipsoidal particle - that the Nusselt number is the same as an equivalent
spherical particle at Reynolds number of 10 but starts to differ as the Reynolds number
increases. They reported that when the Reynolds number is greater than 10, the Nusselt
number of an isolated ellipsoidal particle is lower than the equivalent spherical particle when
the ellipsoid is oriented in a streamwise direction (major axis aligned with flow) and higher
when orientated perpendicular to the flow (minor axis aligned with flow). In the random
assemblies studied here, there are very few particles with major axis aligned to the flow and
thus for Re>10, the predicted Nusselt numbers are consistently higher than spherical
assemblies. Figure 3.14 shows the mean value of Nusselt number vs Reynolds number at
different solid fractions. Both ellipsoids and spheres have a sublinear dependence on
Reynolds number, but ellipsoidal particles show a larger increase with Reynolds number than
spherical particles. Similar trends have also been reported for single isolated particles, the
influence of particle shape on Nusselt number increases as Reynolds number increases [61].

To get a good estimate of Nusselt number for ellipsoid particles, the following
correlation is proposed to fit the current simulation results:

\[
Nu = (1.49 - 0.885\epsilon + 0.078\epsilon^2)(2.458 - 0.042Re^{1.09}Pr^{1/3}) \\
+ (1.114 - 0.62\epsilon - 0.08\epsilon^2)Re^{0.7}Pr^{1/3}
\]

\text{Equation 3.15}

where \(\epsilon\) is the void fraction, \(\epsilon = 1 - \phi\). This correlation is based on the form proposed by
the Gunn correlation, but with modified coefficients to accommodate the current data. The
correlation fit with the simulation data is shown in Figure 3.13 and Figure 3.14. The average
difference between the correlation and the data is under 3%, calculated using

\[
\text{diff} = \frac{1}{n} \sum_{i=1}^{N} \left| \frac{Nu_{eq,i} - Nu_{PRS,i}}{Nu_{PRS,i}} \right|
\]

The correlation in Equation (15) is also valid as the solid fraction \(\phi \to \)
The prediction of Nusselt number from Equation (15) agrees well with the data in [61] for an isolated ellipsoidal particle at any orientation when the Reynolds number is low \((Re \leq 50)\). As the Reynolds number increases beyond 50, the orientation of the particle cannot be neglected and the Nusselt number now becomes dependent on the orientation. However, the dependence is not very strong and Equation (15) still gives a reasonable estimate. In general, the current correlation is valid for the ellipsoidal particle with geometry parameters shown in Table 3.1 in the range \(10 \leq Re \leq 50\) for solid fraction of \(0 < \phi \leq 0.35\), and \(50 \leq Re \leq 200\) for solid fraction of \(0.1 \leq \phi \leq 0.35\).

### 3.6 Summary and Conclusions

In this study, Particle-Resolved Simulations (PRS) are performed to study the heat transfer in flow through a fixed random assembly of spherical particles and ellipsoidal particles in the range of \(10 \leq Re \leq 200\) and \(0.1 \leq \phi \leq 0.35\). The random particle assembly, with 191 to 669 particles based on the solid fraction, is generated using a physics simulation engine SDK- PhysX. The particle-fluid boundaries are resolved using the Immersed Boundary Method (IBM) with constant heat flux boundary conditions. For each solid fraction and Reynolds number, simulation results are averaged based on three different random configurations. Nusselt numbers for spherical particles are compared with the widely used Gunn correlation and other particle resolved simulation data from the literature. The current predictions show good overall agreement with Sun et al.’s particle resolved simulation data but discrepancies do exist. Possible reasons for these discrepancies are discussed. The model is then applied to an assembly of ellipsoidal particles. Simulation results show that the local
velocity and temperature field are significantly affected by the particle orientation. Nusselt number for ellipsoidal particles are not substantially different from spherical particle assemblies at low Reynolds numbers less than 10, but the differences increase as the Reynolds number increases to 200. Finally, a Nusselt number correlation for the ellipsoidal particle geometry is proposed based on the simulation data. The proposed correlation is valid for the ellipsoidal particles of aspect ratio 1:2.5 in the range $10 \leq Re \leq 50$ for solid fraction of $0 < \phi \leq 0.35$, and $50 < Re \leq 200$ for solid fraction of $0.1 \leq \phi \leq 0.35$.

### 3.7 Acknowledgements

Danesh Tafti would like to acknowledge Dr. Mehrdad Shahnam, National Energy Technology Laboratory (NETL), whose support through the ORISE Faculty program was crucial to this project. The authors acknowledge Advanced Research Computing at Virginia Tech for providing computational resources and technical support that have contributed to the results reported within this paper. URL: [http://www.arc.vt.edu](http://www.arc.vt.edu).
3.8 Nomenclature

\( A \) area

\( d \) distance

\( D_{eq} \) equal volume sphere diameter

\( F \) normalized force

\( h \) heat transfer coefficient

\( k \) thermal conductivity

\( L \) length

\( N \) number of particles

\( \text{Nu} \) Nusselt number

\( n \) surface normal

\( P, p \) pressure

\( Pr \) Prandtl number

\( Re \) Reynolds number

\( t \) time

\( u \) streamwise interstitial velocity

\( U \) superficial flow velocity

Greek

\( \alpha \) angle describing ellipsoidal particle orientation

\( \beta \) mean pressure gradient constant

\( \epsilon \) void fraction
\( \rho \)  
\( \mu \)  
\( \phi \)  
\( \psi \)  
\( \tau \)  

**Subscripts**  
\( e \) surface element  
\( IS \) immersed surface  
\( p \) probe  

**Superscripts**  
\( * \) dimensional value  

**Miscellaneous**  
\( x, y, z \) Cartesian coordinates
### 3.9 Tables

Table 3.1. Particle shape parameters and the number of particles for each solid fraction.

<table>
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<tr>
<th>Shape parameter</th>
<th>Sphere</th>
<th>Ellipsoid</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diameter = 1</td>
<td></td>
<td>Semi-major 0.921</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Semi-minor 0.368</td>
</tr>
<tr>
<td>Sphericity</td>
<td>1</td>
<td>0.887</td>
</tr>
<tr>
<td>(D_{eq})</td>
<td>1</td>
<td>1</td>
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<table>
<thead>
<tr>
<th>Number of particles ((N))</th>
<th>(\phi = 10%)</th>
<th>(\phi = 20%)</th>
<th>(\phi = 30%)</th>
<th>(\phi = 35%)</th>
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<td>669</td>
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Table 3.2. Nusselt number from grid independence study for spherical particles in assembly at solid fraction of 0.1

<table>
<thead>
<tr>
<th>Re</th>
<th>Nusselt number (Nu)</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>10</td>
</tr>
<tr>
<td></td>
<td>Mean</td>
</tr>
<tr>
<td>30 cell per $D_{eq}$</td>
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</tr>
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<td>40 cell per $D_{eq}$</td>
<td>3.68</td>
</tr>
<tr>
<td>50 cell per $D_{eq}$</td>
<td>3.73</td>
</tr>
</tbody>
</table>
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Figure 3.6. Temperature of the immersed particle surfaces at solid fraction of 20%, Reynolds number of 200. (a) quarter front view; (b) quarter back view; (c) partial enlarged detail.
Figure 3.7. Spherical particle assembly at solid fraction of 20%, Reynolds number of 200: (a) Average temperature of the particle surface (Equation 3.13) and mixed mean temperature (Equation 3.14) vs X-axis; (b) Nusselt number vs X-axis.
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Figure 3.10. Temperature at the immersed surface of ellipsoidal particles at solid fraction of 20%, Reynolds number of 200. (a) quarter front view; (b) quarter back view; (c) partial enlarged detail.
Figure 3.11. Ellipsoidal particle assembly at solid fraction of 20%, Reynolds number of 200: (a) Average temperature of the particle surface (Equation 3.13) and mixed mean temperature (Equation 3.14) vs X-axis; (b) Nusselt number (Equation 3.15) vs X-axis
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Chapter 4

Variation of drag, lift and torque in an assembly of ellipsoidal particles

4.1 Abstract

Previous research has mostly been focused on the drag force in fluid-particle assemblies. However, when the particle geometry is non-spherical, secondary forces and torque may no longer be negligible. In this study particle-resolved simulations are performed to study the drag force, other secondary forces, and torque in flow through a fixed random assembly of ellipsoidal particles with sphericity ($\psi = 0.887$). The incompressible Navier-Stokes equations are solved using the Immersed Boundary Method (IBM). The assembly of ellipsoidal particles is simulated for solid fraction between 0.1 to 0.35 using 191 to 669 particles, respectively, at low to moderate Reynolds numbers ($10 \leq Re \leq 200$). The results show that the mean drag and lift force and torque variations with flow incidence angle on individual particle follow trends similar to that found for isolated particles. However, there are large variations in these quantities under the same conditions of Reynolds number, void fraction, and incidence angle which become more significant as the Reynolds number increases, leading to the conclusion that local flow conditions in the assembly have a large impact on forces and torques experienced by a particle. Comparing the ratio of secondary lift and lateral forces to the drag force on each particle at the same Reynolds number and solid fraction, shows that approximately 80% of particles for lift and 60% for lateral force are within 10% of the drag force at low Reynolds numbers, but a significant number of particles exhibit values greater than 10% (70% for lift and 50% for lateral force) as the Reynolds number increases, leading to the conclusion that neglecting secondary forces can
introduce substantial errors. As expected, the mean value of torque coefficient increases with void fraction and decreases with Reynolds number. However, individual particles at the same mean flow conditions show large variations about the mean, even acting in the opposite direction to that indicated by the mean value.

4.2 Keywords:
Particle resolved simulations; assembly of non-spherical particle; ellipsoid; drag force; lift force; torque.

4.3 Introduction
Dense gas/liquid-solid flow are fundamental to many industrial processes such as pollution control, separation technologies, CO2 capture, biomass gasification, chemical reactors, sprays, dryers, pneumatic conveying, erosion and sedimentation, etc. In order to have better understanding of the inter-phase momentum transfer in such flows, extensive experimental and numerical studies have been carried out during the last several decades. Most of the studies have focused on spherical particle shapes to simplify the challenge of understanding the flow and particle characteristics. However, in most natural and industrial processes, the particle shape is seldom spherical. For non-spherical particles, as new degrees of freedom are introduced to the system, packing and flow structure are affected which are critical to momentum, heat and mass transfer between particles and fluid. Although the importance of particle shape has been widely recognized, only a few drag models in the literature are suitable for this purpose.
Most research on drag coefficient for non-spherical particle have focused on a single isolated particle. Many studies have been devoted to develop a single general correlation for prediction drag force which covers a number of different particle shapes. Chhabra et al. [7] studied correlations for estimating the drag coefficient of non-spherical particles in incompressible viscous fluids. 1900 experimental data points from 19 independent studies were used to evaluate the accuracy of five correlations, including those proposed by Haider and Levenspiel [8], Ganser [9], Chien [10], Hartman et al. [11] and Swamee and Ojha [12]. They found that the correlation developed by Ganser, which takes the equivalent spherical diameter and the sphericity as the particle shape parameters, has the most accurate prediction. The average error from this correlation was 16%, though the maximum error was as high as 180%. Holzer and Sommerfeld [13] proposed a general drag correlation which depends on particle sphericity, Reynolds number, and particle orientation. Comparing to 2061 experimental data points, they showed that the new correlation had a mean relative deviation of 14.1%. Other than the general correlations, several correlations have also been proposed for certain particle shape and orientation. Zastawny et al.[41] proposed correlations for drag, lift and torque coefficient based on DNS results of non-spherical particle. Four different particle geometries are studied, and the particle fluid boundary is resolved using immersed boundary method. The correlations rely on the angle of incidence between the principle axis of the particle and the fluid velocity and the Reynolds number. They found that early literature provides relatively good predictions for drag coefficient while the predictions for both lift and torques have poor accuracy. Ouchene et al.[69] studied the drag, lift, and pitching torque for ellipsoid particles with three different aspect ratios using direct numerical simulation(DNS) for Reynolds number ranging from 0.1 to 290. They found the drag correlations proposed by Zastawny et al.[41] agreed best with their DNS results compared to correlations developed by Rosendahl [70] and Holzer and Sommerfeld [13], while still having a mean deviation of 20%. They also found that the lift force is mainly contributed by the
pressure force irrespective of aspect ratio, angle of incidence, and Reynolds number. Their lift force results showed between 2% to 25% difference compared to the lift force correlation developed by Zastawny et al.[41]. They suggested that further efforts are necessary to develop more accurate correlations for drag, lift and torque coefficients. Sanjeevi and Padding[71] examined the drag force and lift force for prolate (needle-like) and oblate (disc-like) spheroids using lattice Boltzmann method. They found that the sine-squared drag law $C_{D,\phi} = C_{D,\phi=0^o} + \left( C_{D,\phi=90^o} - C_{D,\phi=0^o} \right) \sin^2 \phi$ holds up from low to high Reynolds numbers ($Re = 2000$) for prolate spheroids. Their results demonstrate that the drag coefficient for such particles at an arbitrary incidence angle can be obtained based on just two simulations at $\phi = 0^o$ and $\phi = 90^o$ for a given Re. However, the oblate spheroid with aspect ratio of 4 or larger does not follow this drag law due to strong wake-induced drag. They also found that for lift force, the theoretical equation $C_{L,\phi} = \left( C_{D,\phi=90^o} - C_{D,\phi=0^o} \right) \sin \phi \cos \phi$ can give a reasonable estimate even at high Reynolds number for prolate spheroids. Among researches about stationary particles, Auguste et al.[72], Shenoy et al[73] and Yang [74] studied transient drag, lift and bifurcations of low aspect ratio (less than 1) cylinders with axis of rotational symmetry parallel to fluid velocity. For particles inclined to flow field, research has been done about slightly inclined cylinder of aspect ratio 1/6 [75]. Computational simulation of Vakil and Green [76] studied lift and drag on cylinders with aspect ratio larger than 2 at different inclination angle.

For non-spherical particles in an assembly, all past studies have focused on the drag force. Nemec and Levec [17] demonstrated that the original Ergun equation [3] systematically under-predicts the pressure drop in flow over non-spherical particles. They proposed that the constants in the dimensionless form of the Ergun equation, developed by Niven [18], should be modified based on particle shapes. They conclude that with their modifications, the Ergun equation is able to predict pressure drop in flow through a packed bed of cylinders, rings and polylobes within 10% error.
However, there is no correlation to calculate the constants for arbitrary particle shapes, leaving that determination to experiments or particle resolved simulations. Moreover, the original Ergun equation significantly over-predicts the average drag force at low solid volume fractions [19], and hence the modified equation of Niven applied to a dilute system of non-spherical particles has not been validated. Hilton et al.[77] introduced a method to couple DEM simulations of non-spherical particles to a new pressure gradient force Navier–Stokes formulation and investigated the behavior of non-spherical particles in a three-dimensional fluidized bed. Their results showed that particle shape has significant impact on systems in which particle motion is coupled to fluid flow, and must be taken into account to correctly determine the dynamics of these systems. Machač and Dolejš [20] investigated the pressure drop in flow through a random fixed bed of non-spherical particles. They suggested that a ‘bed factor’ which contains the information of the non-spherical particle surface area is needed to accurately predict the pressure drop. Vollmari et al.[24] studied pressure drop in densely packed fixed bed with non-spherical particles. Experiments and DEM simulations were performed to evaluate the accuracy of drag correlations. They found that the pressure drop can only be addressed by considering the particles’ orientation, and an average of 50% deviation in pressure drop is observed between DEM and experimental data if orientation is not considered. They recommend fully resolved simulations to understand the effects of inhomogeneous packing on fluid flow structure introduced by the non-spherical particle shape. Hua et al.[21] studied the combined Ganser and Ergun correlations and modified Syamlal and O’Brien drag models in a Eulerian-Eulerian CFD framework for irregular shaped particles in dense gas-solid fluidized beds. Zhou et al. [23] studied packed ellipsoidal particles in a fluidized bed using CFD-DEM simulations. The drag model developed by Holzer et al. [13] was used for the ellipsoids. They concluded that the accuracy and applicability of current correlations is questionable, and a general and reliable correlation to determine fluid drag on non-spherical particles is urgently needed. In He et al.[50], three categories of drag correlation were
evaluated against particle resolved simulation of ellipsoidal particles in assembly. The results showed that the mean drag force of ellipsoidal particle with aspect ratio of 2.5 is 15% to 35% larger than equal volume spherical particles at the same solid fraction and Reynolds number. They also found that drag correlations which have particle orientation as a parameter have better performance than other correlations.

In summary, for isolated single non-spherical particles, there are limited number of general drag force correlations available. Lift and torque correlations have been proposed for certain particle shapes, but no general correlation is available. For particles in assembly, limited number of studies have been carried out to predict the drag force, while markedly scarce information is available for predicting lift force, lateral force, and torque. All these studies demonstrate that further investigation is needed to have a better understanding of flow through an assembly of non-spherical particles. Therefore, in this study, particle-resolved simulations are carried out to investigate drag, lift force, lateral force and torque for a random assembly of non-spherical particles. In this approach, fluid force and torque on each particle is calculated by resolving the flow field around each individual particle. Ellipsoidal particles with aspect ratio of 2.5 are used and the particle-fluid boundaries are resolved using an Immersed Boundary Method (IBM). The objectives of the current study are: 1. quantitatively compare the variation of lift force and lateral force compared to the drag force in the fluid particle system; 2. compare the torque coefficient in assembly to that of a single isolated particle; 3. based on the numerical results, provide guidance for reduced order simulations.

4.4 Governing Equations and Methodology

All simulations are performed using an in-house code – Generalized Incompressible Direct and Large Eddy Simulation of Turbulence (GenIDLEST). The details of the framework and methodology used in GenIDLEST can be found in Tafti [26] and Tafti [27]. In this section, the
relevant governing equations and the modified treatments of the governing equations under fully-developed flow conditions are presented along with some details of the Immersed Boundary Method [28]. GenIDLEST with immersed boundary method has been successfully applied to oscillating cylinders [28], turbine cooling passage heat transfer [29], fluid structure interactions problems [30] and heat transfer in non-spherical particle assembly [78].

4.4.1 Governing Equations and Numerical Technique

The non-dimensional form of the Navier-Stokes equations for incompressible flow are as follows:

Continuity:
\[
\frac{\partial u_i}{\partial x_i} = 0
\]

Equation 4.1

Momentum:
\[
\frac{\partial u_i}{\partial t} + \frac{\partial (u_j u_i)}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{1}{Re_{ref}} \left( \frac{\partial^2 u_i}{\partial x_j \partial x_j} \right)
\]

Equation 4.2

where the non-dimensionalizations are:

\[
x_i = \frac{x_i}{L_{ref}}; \quad u_i = \frac{u_i}{u_{ref}}; \quad t = \frac{t^* u_{ref}^*}{L_{ref}}; \quad P = \frac{P^* - P_{ref}^*}{\rho_{ref}^* u_{ref}^*}; \quad Re_{ref} = \frac{\rho_{ref} u_{ref}^* L_{ref}^*}{\mu_{ref}^*}
\]

The above governing equations are transformed to generalized coordinates, and discretized in a conservative finite-volume formulation using a second-order central (SOC) difference scheme on a non-staggered grid topology [31]. Cartesian velocities, pressure and temperature are calculated and stored at the cell center, whereas fluxes are calculated and stored at cell faces. A projection method using second order predictor-corrector steps is used for the time integration of the continuity and momentum equations. In the predictor step, an intermediate velocity field is calculated; and in the
corrector step, an updated divergence free velocity is calculated at the new time-step by solving a pressure-Poisson equation.

4.4.2 Fully developed calculations

The computational domain consists of a three-dimensional periodic box representing an unbounded particle assembly. Flow is induced along the x-direction by applying a constant mean pressure gradient to balance the form and friction losses, and the total pressure is expressed in terms of the mean pressure and a fluctuating or periodic component as shown in Equation 4.3

\[ P(\vec{x}, t) = -\gamma \cdot x + p(\vec{x}, t) \]  \hspace{1cm} \text{Equation 4.3}

where \( \gamma \) is a constant. Because the applied pressure gradient will balance the form and friction losses when the flow reaches a steady state, the actual value used for \( \gamma \) is not of any consequence to the calculated forces as long as the mean Reynolds number obtained from the simulation is the same.

With the unchanged continuity equation, the momentum equation can be written as:

\[ \frac{\partial u_i}{\partial t} + \frac{\partial (u_j u_i)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{1}{Re_{ref}} \left( \frac{\partial^2 u_i}{\partial x_j \partial x_j} \right) + \gamma \vec{e}_x \]  \hspace{1cm} \text{Equation 4.4}

The \( \gamma \vec{e}_x \) in Equation 4.4 is the mean applied pressure gradient source term, which balances the mean form and friction losses in the flow direction. The detailed procedure used can be found in Patankar [32] and Zhang et al. [33].

4.4.3 Immersed Boundary Method (IBM)

The immersed boundary method (IBM) used in this paper is an indirect forcing sharp interface approach. This method is an extension of a scheme originally proposed by Gilmanov and Sotiropoulos [34], and has been modified to fit the generalized coordinate system and non-staggered grid framework of GenIDLEST. In this method, the governing equations are solved without modification for the computational grid in the fluid domain. Special treatment is only applied to the
first layer of the fluid nodes (fluid IB nodes) next to the immersed boundary. The detailed implementations of IBM can be found in Nagendra et al. [28].

**Force:**

The fluid force is calculated on each surface element of the immersed surface which is defined by an unstructured triangulated mesh. The immersed surface of the ellipsoidal particles used in the current simulation is shown in Figure 4.1(a). 2172 unstructured triangle surface elements are used to represent the surface mesh. Fluid force due to pressure and shear are separately calculated on each elements.

\[
\vec{F}_e = \vec{F}_{\text{pressure}} + \vec{F}_{\text{visous}} \quad \text{Equation 4.5}
\]

The total fluid force on each particle is obtained by:

\[
\vec{F}_{f-p} = \sum_{i=1}^{n} \vec{F}_{e,i} \quad \text{Equation 4.6}
\]

Where \( n \) is the total number of triangular elements on each particle.

The details of force calculation can be found in He et al.[50].

**Torque:**

In the current simulations, torque for each particle is calculated with respect to its geometric center.

The torque from the fluid force on each triangle surface element is calculated using:

\[
\vec{T}_e = \vec{r} \times \vec{F}_e \quad \text{Equation 4.7}
\]

\( \vec{r} \) is the vector from the particle geometric center to the triangular surface element centroid, shown in Figure 4.1(b).

The total torque for each particle can be obtained by:
\[
\vec{T}_{f-p} = \sum_{i=1}^{n} \vec{T}_{e,i}
\]

Equation 4.8

Because \( \vec{F}_e \) is the sum of \( \vec{F}_{\text{pressure}} \) and \( \vec{F}_{\text{visous}} \), torque \( \vec{T}_{f-p} \) has the contribution from both fluid pressure force and viscous force.

4.5 Computational Details

4.5.1 Geometry, Grid and Simulation Parameters

The computational setup in the current simulation is the same as that published earlier in He et al.\[50\]. In the present study, only a mono-disperse fluid particle system is considered, i.e. all particles have the same geometric parameters. The computational domain is a cube, with the periodic boundary condition applied along all three directions. A pressure gradient is applied along the x-direction to drive the fluid flow, as discussed in section 2.2. Particles are randomly distributed in the computational domain, fixed at their initial positions. In all calculations, \( U_{\text{ref}} = U \), the superficial velocity which equals the x-direction volumetric flowrate divided by the area of the cross-section, and \( L_{\text{ref}} = D_{eq} \), the equivalent spherical diameter. Thus the Reynolds number is defined as:

\[
Re = \frac{\rho U D_{eq}}{\mu}
\]

Equation 4.9

where \( \rho \) and \( \mu \) are the fluid density and dynamic viscosity.

When the flow reaches a steady state, fluid forces and torque acting on each particle are calculated. By averaging the forces and torque over all the particles in the fluid domain, the drag force is calculated for a given Reynolds number and solid fraction. Similar methods have already been successfully used to extract drag laws for spherical particles in assembly by Hill et al. \[35\], Van Der Hoef et al. \[37\], Beetstra et al. \[38\] and Tenneti et al. \[36\].
The computational domain is a cube with side $10D_{eq}$, with the center of the computational domain located at origin $(0, 0, 0)$. A grid independency study is carried out with resolutions of 30, 40, and 50 background grid cells per equivalent particle diameter. A random realization of ellipsoidal particle assembly at 0.1 solid fraction is chosen as the test case. Fluid forces and torque are recorded when the flow reaches a steady state. The results show that the maximum difference between the three grids is about 2% so 40 grid cells per $D_{eq}$ were deemed to be sufficiently fine to resolve the fluid field around each particle[50].

Because of the fixed domain size, the number of particles, $N$, in the computation domain is a function of solid volume fraction $\phi$ alone:

$$N = \frac{6\phi L^3}{\pi D_{eq}^3} = \frac{6000\phi}{\pi}$$

Equation 4.10

Sphericity $\psi$, proposed by Wadell [39] is the most widely used parameter to quantify the shape of non-spherical particles.

$$\psi = \frac{1}{\pi} \left(\frac{6V_p}{A_p}\right)^{\frac{2}{3}} = \frac{A_s}{A_p}$$

Equation 4.11

where $A_p$ is the surface area of the particle, $V_p$ is the volume of the particle, and $A_s$ is the surface area of a sphere which has the same volume as the particle. The more spherical a particles is, the closer this factor gets to one. The geometry parameters and number of particles for each solid fraction are shown in Table 4.1. An ellipsoidal particle shape is chosen because CFD-DEM simulation methods have been developed for such particles[23][79], but the drag correlations used in these studies are not validated, and the secondary forces and torque from the fluid are neglected. In addition, the drag coefficient for a single isolated ellipsoidal particle as a function of particle orientation and Reynolds number is available in the literature [41]. For solid fraction of 0.1, 191 particles are used which increase to 669 particles for $\phi=0.35$. To increase the sample size for the current simulations, three
random realizations of particle assembly are tested for each solid fraction. Forty-eight cases (3 realizations, 4 Reynolds number, 4 solid fraction) are simulated in total. In contrast, past particle resolved simulation studies on assembly of particles have used 32 to 60 particles [35], 54 particles [37][38], 16 to 161 particles [36] for solid fraction between ~0.1 to ~0.5. The solid fraction for ellipsoids was limited to 0.35 because beyond this packing density it became difficult to generate a random distribution without particle-particle overlap. To generate distributions with higher solid fractions it would have been necessary to give some preferential orientation to the ellipsoids and would have been outside the scope of this investigation.

Each simulation uses 400 × 400 × 400 background computational cells in the X, Y and Z directions, respectively, for a total cell count of 64 million. The calculations are run on 100 processing cores and a typical calculation takes 40 wall clock hours to converge to the final solution.

The mean value at each solid fraction is calculated using the following equation:

\[ \bar{\chi} = \frac{1}{N} \sum_{i=1}^{N} \chi_i \]  

Equation 4.12

Where \( \chi \) is the fluid force or torque on each particle, \( N \) is the total number of particles simulated at each solid fraction and Reynolds number.

4.5.2 Particle Assembly

The random particle assembly is generated using a physics simulation engine SDK- PhysX by Nvidia [42]. During the assembly process, each particle is randomly spawned in the designated space and associated with a mesh to represent its geometry. If the particle spawns at a location which has already been occupied by another particle, an overlap is detected between the convex meshes associated with each particle, and these two particles are relocated. This process ensures that a random assembly of particles is created with no overlap. Any shape with a CAD file format can be
imported and packed in this framework. After the assembly, the location and orientation of each particle is used to create the surface mesh for IBM.

4.5.3 Global and local coordinate system

A local coordinate system \((X', Y', Z')\) associated with each particle is introduced to conveniently describe the force and torque, as shown in Figure 4.2(a). The \(X'\) axis is parallel to the fluid-particle relative velocity. In the current simulations, the mean flow is in the \(X\) direction imposed by the pressure gradient applied in \(X\) momentum equation, therefore, \(X'\) in the local coordinate is aligned with the global \(X\) axis. The \(Y'\) axis is defined as: (1) normal to \(X'\) axis; (2) in the plane formed by the \(X'\) axis and the principle axis of the particle (semi-major axis of the ellipsoid); (3) keeping the angle \(\alpha\) in the first quadrant of \(X'Y'\) coordinates. The angle \(\alpha\) is defined as the angle between the relative velocity and the principle axis of the particle. The \(Z'\) axis is normal to \(X'\) and \(Y'\) and follows the right-hand rule. Because \(X'\) is parallel to \(X\), the angle \(\beta\) between \(Y'\) and \(Y\) is enough to define the transformation matrix from global coordinates to local coordinates, as shown in Figure 4.2(b). In rare cases, when the principle axis of the particle is aligned with flow direction, the local and global coordinate systems are identical.

The fluid force on each particle is decomposed in the local coordinate system: drag force, \(F_D\), is the fluid force in the \(X'\) direction; Lift force, \(F_L\), is the fluid force in the \(Y'\) direction; lateral force, \(F_{LAT}\), is the fluid force in the \(Z'\) direction. Torque due to fluid force is also decomposed in the local coordinate system.

4.5.4 Non-dimensionalization

In accordance with previous work in the literature[50], all forces are normalized using the Stokes-Einstein relation:
\[ F = \frac{F_{f-p}}{3\pi \mu D_{eq} U} \]  \hspace{1cm} \text{Equation 4.13}

Torque coefficient is defined by:

\[ T = \frac{T_{f-p}}{\sum \rho U^2 \frac{\pi}{8} D^3_{eq}} \]  \hspace{1cm} \text{Equation 4.14}

\section*{4.6 Results and Discussion}

The surface mesh of each ellipsoidal particle is an unstructured mesh consists of 2172 triangular elements, shown in Figure 4.1(a). Four different solid fractions \( \phi \), ranging from 0.1 to 0.35, are tested. Reynolds number based on the superficial velocity and diameter are tested at 10, 50, 100 and 200. Drag force, lift force, lateral force and torque on each particle is calculated when the fluid field reaches a steady state.

Figure 4.3(a) shows the surface mesh created based on assembly information from PhysX. Figure 4.3(b) shows the immersed surface identified by GenIDLEST for an assembly with solid fraction of 0.2. In Figure 4.3(b), some particle surfaces are cut by the fluid grid boundary, this is because the periodic boundary condition is applied to both fluid computational grid and immersed surface for particles. When a particle is located across the fluid periodic boundary, the surface mesh of the particle located in the computational domain remains at its original location, while the other part outside the computational domain is relocated to the corresponding periodic side.

Figure 4.4 shows the non-dimensional interstitial u-velocity in the assembly of ellipsoidal particles at a solid fraction of 0.2 and Reynolds number of 100. The velocity magnitude is dependent
on the local particle packing density with larger fluid velocities prevailing in regions with smaller interstitial spaces.

4.6.1 Drag force

For particles in assembly, both the orientation and the location of neighboring particles with respect to the approach flow have a large impact on the drag force, or for that matter, on all forces and torque, acting on any given particle. This is illustrated in Figure 4.5 for the drag force. In Figure 4.5(a), the ellipsoid is oriented at an angle of 1.15 radians (66°) to the flow with a drag force of 7.69, whereas the ellipsoid in Figure 4.5(b) is oriented at 0.11 radians (6°) angle but still exhibits a large force of 6.7. Conversely, Figure 4.5(c) shows a particle at approximately the same angle as in (a) but it experiences a much smaller drag force of 3.59. This is because the neighboring particle orientations and relative locations have a large effect on the velocity field which impacts the drag force. For example, the particle in Figure 4.5(c) lies in the wake region of upstream particles, whereas the particle in Figure 4.5(b) experiences accelerated flow. For reference, for an ellipsoid in isolation, the corresponding drag forces are 1.72 and 1.25 for a particle oriented at 1.15 radian and 0.11 radian, respectively.

In Figure 4.6, the mean non-dimensional drag force at different solid fractions is plotted against the Reynolds number. The mean drag force is calculated based on Equation 4.12. At a given solid fraction, the non-dimensional drag force shows a nearly linear increase as the Reynolds number increases. At a given Reynolds number, the drag force also increases as the solid fraction increases. This is because while the Reynolds number is based on the superficial velocity, the effective local Reynolds number for each particle is defined by the interstitial velocity field which increases in the mean as the solid fraction increases, thus increasing the mean drag force.
In Figure 4.7, drag force at each solid fraction is plotted against the Reynolds number. The bars in the plot are the standard deviation of the drag force, showing the variability of the drag force on each particle with respect to the mean drag force. At the same solid fraction, the standard deviation increases as the Reynolds number increases. The relative standard deviation (standard deviation/mean, also known as the coefficient of variation) of the drag force is about 0.15 at Reynolds number of 10, indicating that 68% of the particles in assembly have drag force in the range of 0.85 to 1.15 of the mean drag force with 32% falling outside this range. At Reynolds number of 200, the relative standard deviation increases to about 0.35, suggesting that 68% of the particles have drag force in the range of 0.65 to 1.35 of the mean drag force, while 32% of the particles have drag forces either smaller than 0.65 of the mean drag force or larger than 1.35 of the mean drag force. This result suggests that current widely used drag force correlations which only estimate the mean drag force can introduce large errors when applied to an individual particle in an assembly.

The contribution to fluid drag force on each particle is from two sources: from pressure force and from viscous force. Figure 4.7 also shows the contributions from pressure and viscous drag, normalized by the Stokes-Einstein relation at different solid fractions. For all solid fractions, the pressure force increases linearly with the Reynolds number while the viscous force varies at a sublinear power of the mean flow Reynolds number. The contribution from pressure force becomes dominant as the Reynolds number increases to 200. At the same time, the pressure force increases more significantly than the viscous force as solid fraction increases. At a solid fraction of 0.1, the viscous force contributes more than 50% of the drag force when Reynolds number is less than or equal to 50, and decreases to about 33% at Reynolds number of 200. While at solid fraction of 0.35, the viscous force is always less significant than pressure force, contributing about 40% at Reynolds number of 10, while decreasing to 20% at Reynolds number of 200.
Figure 4.8 and Figure 4.9 shows the drag force on each individual particle against the particle incidence angle $\alpha$ (shown in Figure 4.2) at solid fraction of 0.1 and 0.35. The figures in the left column show the total drag force: the blue points is the total drag force on each particle, and the red points are the averaged drag force of particles in every 0.1 radian. The figures in the right column are the drag force from pressure and viscous forces on each particle. Data from all three different random assembly configurations are plotted in this figure, therefore, 571 data points are recorded for solid fraction of 0.1 and 2007 points for solid fraction of 0.35.

At solid fraction of 0.1 and Reynolds number of 10, although the total drag force doesn’t show significant variation with increase in incidence angle, the viscous force and pressure force have clear opposite trends with the change in incidence angle. The pressure force increases because the projected area of the ellipsoid particle in the mean flow direction increases as the incidence angle increases. Conversely, the projection of the area over which shear stress contributes to drag, decreases. The viscous force contributes about 75% of the drag force at low incidence angle, but decreases to about 50% at high incidence angle. At solid fraction of 0.1 and Reynolds number of 200, the increment in pressure force with incidence angle is significant and the total drag force is dominated by the behavior of the pressure field. The variation of pressure and viscous force with the change in incidence angle is very similar to an isolated ellipsoidal particle[71], although the magnitude of force change is much larger in the assembly. Another feature of the behavior of drag force in assembly is the large variation in force at a given incidence angle.

To quantify the variation of forces at each incidence angle, a sensitivity parameter $\lambda$ is defined as:

$$
\lambda(\alpha) = \frac{\max(F(\alpha)) - \min(F(\alpha))}{\frac{1}{2} (\max(F(\alpha)) + \min(F(\alpha)))}
$$

**Equation 4.15**
At solid fraction of 0.1, for the pressure force, $\lambda$ increases from $\sim60\%$ to $\sim100\%$ as the incidence angle increases from 0 to $\pi/2$, suggesting that a particle aligned at near $90^\circ$ to the flow is much more sensitive to the flow induced by neighboring particles. Moreover, although the pressure force magnitude increases, $\lambda$ does not show significant variation as the Reynolds number increases. For viscous forces, $\lambda$ is independent of the Reynolds number and the incidence angle, suggesting that flow perturbations imposed by neighboring particles do not have a significant impact on the viscous drag force.

At solid fraction of 0.35, similar but stronger trends are observed in the pressure and viscous force contributions. Pressure has a much larger overall contribution to total drag than viscosity for all Reynolds numbers and incidence angles. As the Reynolds number increases, pressure force becomes the main contributor to drag force. For pressure force, the sensitivity parameter, $\lambda$, increases as the incidence angle increases, from $\sim20\%$ to $\sim110\%$. Compared to void fraction of 0.1, this observation implies that at high solid fraction, when the incidence angle is small, the pressure force variation is not highly affected by the neighboring particles; however, when the particle is aligned normal to the mean flow direction, the difference in the local flow field has much larger impact on the pressure force. Compared to the pressure force, the variation in viscous force at 0.35 solid fraction is much smaller, leaving $\lambda$ independent of the Reynolds number and incidence angle. The variation in the total drag force is mainly from the pressure force.

4.6.2 Lift force

In reduced-order simulations such as CFD coupled to DEM, one simplification in simulating spherical particles is that once the relative velocity is obtained, the force calculated on the particle is mainly the fluid drag force in the direction of relative velocity while other fluid forces can be neglected. For non-spherical particle, this simplification may not be valid. Taking the ellipsoidal
particle studied in the current paper as an example, the relative mean flow direction is along the X axis, as shown in Figure 4.2(c), but because of the orientation of the particle with respect to the flow direction, there will be an additional lift force acting on the particle in the Y’ direction. This lift force, together with the drag force in the X direction, will push the particle downward and forward.

Figure 4.10 shows the variation of non-dimensional mean lift force with Reynolds number for ellipsoidal particles in assembly at different solid fractions. In the local coordinate system (Figure 4.2), the pressure lift force always acts in the negative Y’ direction. For the Reynolds number range tested in the present study, the magnitude of the pressure force is always larger than that of the viscous force, thus always yielding a negative lift force. The lift force at all solid fractions increases at a super-linear power of Reynolds number. Similar to the fluid drag force, the magnitude of lift force also increases as the solid fraction increases. At Reynolds number of 10, the lift at 0.35 solid fraction is about 300% larger than at 0.10 solid fraction. At Reynolds number between 50 to 200, the lift at 0.35 solid fraction is 150% larger than 0.10 solid fraction, 60% larger than 0.20 solid fraction, and 20% larger than 0.30 solid fraction.

Figure 4.11 shows the variation of the mean lift force and contributions from pressure and viscous shear for the range of Reynolds numbers at different solid fractions. The bars in the plot are the standard deviation of the lift force, showing the variability of the lift force on each particle with respect to the mean lift force at the given Reynolds number and solid fraction. Similar to the drag force, the relative standard deviation also increases as the Reynolds number increases with a high value of 0.8 at Reynolds number of 200.

For all solid fractions, the viscous force is positive acting against the negative pressure lift force. At the same solid fraction, the magnitude of both pressure and viscous force increase as the Reynolds number increases, but the increase in pressure is much more pronounced than the viscous
contribution. Thus, the variation of mean lift force with Reynolds number is mostly dominated by the variation of pressure force.

Table 4.2 shows the mean lift force compared to the mean drag force for the ellipsoidal particles in assembly. At the same solid fraction, the ratio between the lift force magnitude to the drag force increases as the Reynolds number increases. At 0.1 solid fraction, lift force increases from 5% at Reynolds number of 10 to about 20% at Reynolds number of 200. At the same Reynolds number, both drag force and lift force increase as the solid fraction increases, but the increment in drag force is more significant than the increment in lift force, yielding a decreasing ratio of $F_L/F_D$ as the solid fraction increases. Based on the mean results, at low Reynolds number (Re = 10), the lift force is about 5% of the drag force, and therefore can be neglected in a reduced order DEM calculation to simplify the particle movement calculation. However, at higher Reynolds number, the lift force can be as high as 20% of the drag force, and neglecting it will lead to substantial error in calculating particle trajectories.

Similar to the drag force, Figure 4.12 and Figure 4.13 show total lift force (left column): the blue points stand for the total lift force on each particle, and the red points are the averaged lift force of particles in every 0.1 radian. The red line is the lift force correlation for isolated single ellipsoidal particle proposed by Zastawny et al [8]. Lift force from pressure (right column blue scatter) and viscous shear (right column red scatter) on each particle vs particle incidence angle at solid fraction of 0.1 and 0.35 are also shown in Figure 4.12 and Figure 4.13, respectively. At solid fraction of 0.1 and Reynolds number of 10, the averaged lift force in this study is very similar to the single ellipsoidal particle lift correlation proposed by Zastawny et al [8]. However, as the Reynolds number increases, the lift forces in assembly start to show differences from the correlation; the lift force magnitude in assembly is much larger than that for the isolated particle. The difference with the isolated particle correlation increases as Reynolds number and void fraction increase.
Both mean pressure force and lift force magnitude at incidence angle $\alpha$ follow the following equation:

$$F(\alpha) = 2F_{\alpha=\pi/2} \sin(\alpha) \cos(\alpha)$$  \hspace{1cm} \text{Equation 4.16}

Both pressure and viscous forces have the largest magnitude when the particle has $\pi/4$ incidence angle with the mean flow direction. At the same solid fraction, the increase in viscous forces is much less than the increase in pressure forces as the Reynolds number increases. The variation in the sensitivity parameter, $\lambda$, for viscous forces increases as the incidence angle increases, while pressure forces have the largest value of $\lambda$ at $\alpha = \pi/4$ and nearly the same value at 0 and $\pi/2$. This suggests that the perturbations in the flow field have the largest impact on viscous forces when the particle is oriented at higher incidence angles to the flow. Whereas for pressure forces, the local fluid field variation has the largest impact when the particle has $\pi/4$ incidence angle. Similar to the drag force, the variation in lift force is also mainly due to the variation in pressure force.

Figure 4.14 shows the probability histogram of the ratio between magnitude of the lift force over the drag force on each particle in assembly for solid fractions 0.1 and 0.35. At the same solid fraction, the probability of particles having a large ratio of $|F_{y'}|/F_x$ increases as the Reynolds number increases. At Reynolds number of 10, the probability histograms of 0.1 solid fraction and 0.35 solid fraction exhibit a similar distribution (i.e. ~40% of particles have a ratio less than 0.05 in both), however as the Reynolds number increases, the probability histogram of 0.1 solid fraction is more flat than that for 0.35, indicating that more particles have a relatively large $|F_{y'}|/F_x$ ratio at lower solid fractions. These results confirm the conclusion that were made earlier based on Table 4.2, that for simulating ellipsoidal particles using reduced order methods, the lift force may be neglected at low Reynolds number, but at higher Reynolds numbers, the lift force is significant compared to drag force, and therefore cannot be neglected, particularly at low solid fractions.
4.6.3 Lateral force

As shown in Figure 4.2(b), in the local coordinate system, the particle always has mirror symmetry at any incidence angle to the symmetry plane of X’Y’, thus, the lateral force in the z’ direction (or –z’ direction) only results if the flow and pressure field are non-symmetric. Figure 4.15 and Figure 4.16 show the total lateral force, contributions from pressure and viscous shear on each particle vs particle incidence angle at solid fractions of 0.1 and 0.35. The mean value of the lateral force at all incidence angles is near 0, which suggests that the mean value of the lateral force is not affected by the incidence angle. It also suggests that the sample size of random particle orientations over which the mean is obtained is sufficiently large. However, the variation of the sensitivity parameter, \( \lambda \), for both pressure force and viscous force, increases as the incidence angle \( \alpha \) increases. This is because in the local coordinate system, the particle’s projected area in the flow direction is a function of incidence angle \( \alpha \). The increase in force variation suggests that the variation in local fluid field is more pronounced when it has a larger projected area. Another phenomenon that should be noted is that although the mean lateral force for the assembly is zero, the lateral force can be significant for some particles.

Figure 4.17 shows the probability histogram of the ratio between the magnitude of the lateral force over the drag force on each particle in assembly for solid fractions 0.1 and 0.35. At the same solid fraction, the probability of particles having a large ratio of \( |F_{z'}|/F_x \) increases as the Reynolds number increases. At Reynolds number of 10, 50 and 100, more particles have the ratio of \( |F_{z'}|/F_x \) within 10% at solid fraction of 0.1 than that at solid fraction of 0.35, while at Reynolds number of 200, the ratio of \( |F_{z'}|/F_x \) is nearly the same for both solid fractions. In the context of reduced order calculations, the current results suggest that for low Reynolds number and low solid fraction, most particles have a lateral force within 10% of the magnitude of drag force, and therefore, the lateral
force may be neglected for simplicity. However, at high Reynolds numbers, nearly 40% of the particles have lateral force more than 10% of the drag force, and neglecting these forces will lead to inaccuracy in particle trajectories.

4.6.4 Torque

Since the center of total fluid force acting on the particle may not be at the same location as the centroid of the particle, torques due to this force displacement are generated to rotate the particle. The torque due to fluid forces is calculated in the local coordinate system (X’, Y’, Z’) as shown in Figure 4.2. Results show that the torque in X’ and Y’ directions are 2 to 3 orders of magnitude smaller than the torque in Z’ direction, thus, only the torque in the Z’ direction is discussed here.

Figure 4.18 shows the mean torque coefficient in the Z’ direction (defined in Equation 4.14) versus Reynolds number at different solid fractions. At the same solid fraction, similar to the behavior of drag coefficient for particles in assembly, the torque coefficient decreases as the Reynolds number increases. At the same Reynolds number, particles in high solid fraction assembly have a higher mean torque coefficient; the torque coefficient at 0.35 solid fraction is 100% to 125% larger than it is at 0.1 solid fraction over the entire range of Reynolds number in the current study.

Figure 4.19 shows the torque coefficient in the Z’ direction on each particle vs particle incidence angle at solid fractions of 0.1 and 0.35. The solid red line is the torque coefficient correlation for single isolated ellipsoidal particle proposed by Zastawny et al.[41]. The red points are the averaged torque coefficients of particles in every 0.1 radian. As evident, the torque coefficient for particles in assembly has a similar trend as the single isolated particle: zero torque coefficient at zero incidence angle, then increasing as the incidence angle increases, reaching a peak value at $\pi/4$, and then decreasing to 0 at incidence angle of $\pi/2$. This is where the similarity ends. The peak value of the coefficient for particles in assembly at incidence angle of $\pi/4$ has a much higher value than the
proposed single particle correlation. These differences in magnitude increase with solid fraction suggesting that the torque exerted by fluid forces is more significant at higher solid fraction. Different from the single isolated particle, the torque coefficient of particles in assembly have large variations due to the local fluid field disturbed by other particles. For the single isolated particle, the torque in Z’ direction is always positive, rotating the particle in anti-clockwise direction in the local coordinate system, while this is no longer valid for particles in assembly. In assembly, certain particles can have a negative torque coefficient, rotating the particle in the clock-wise direction, even at $\pi/4$ angle of incidence because the local fluid field is highly disturbed.

The large variations encountered in the torque coefficient with incidence angle are similar to that experienced by the drag and lift forces, but with the added dimension that the direction of torque could also be different from the mean value.

**4.7 Summary and Conclusion**

Previous research has mostly focused on the drag force in fluid-particle assemblies. However, when the particle geometry is non-spherical, secondary forces and torques created due to the particle geometry may no longer be negligible. To the author’s knowledge, no study has been carried out to quantitatively evaluate these secondary forces and torques in an assembly of non-spherical particles. Thus, in this study particle-resolved simulations are performed to study the drag force, secondary forces, and torque in flow through a fixed random assembly of non-spherical particles. Ellipsoidal particles with sphericity ($\psi = 0.887$) are investigated in a periodic cubic domain to simulate an infinite assembly. The incompressible Navier-Stokes equations are solved using the Immersed Boundary Method (IBM). Pressure and viscous forces on each particle are calculated based on the resolved flow field. The assembly of ellipsoidal particles is simulated for solid fraction between 0.1 to 0.35 using 191 to 669 particles, respectively, at low to moderate Reynolds numbers ($10 \leq Re \leq$
Three different random assembly realizations are tested at each solid fraction and Reynolds number. Mean value of drag force, secondary force and torque coefficients are calculated for each Reynolds number and solid fraction. Moreover, the detailed forces and torque coefficient variation caused by disturbed local fluid field and particle incidence angle are also presented.

The following major conclusions can be drawn from this study:

1. Unlike spherical particles, in which force variations are only due to the non-uniform local flow field perturbed by the neighboring particles, the drag, lift force, and torque coefficient for ellipsoidal particles show a clear dependency on the incidence angle of the flow. In the local coordinate system, the variation of mean drag force, lift force, and torque coefficient with incidence angle show trends similar to that of a single isolated particle. However, the magnitude of such variations are much larger for the particles in assembly. Although the mean lateral force is independent of the incidence angle, the variation of lateral force increases as the incidence angle increases.

2. The drag, lift, lateral forces, and torque coefficients are very sensitive to the local flow conditions and exhibit large variations under the same conditions of Reynolds number and void fraction. These variations increase with Reynolds number. For example, for drag force at Reynolds number of 200 (\(\phi=0.1\)), 32% of the particles can have drag forces either smaller than 0.65 of the mean drag force or larger than 1.35 of the mean drag force. Similarly, for lift force at Reynolds number 200 (\(\phi=0.35\)), 32% of the particles can have lift forces either smaller than 0.13 of the mean lift force or larger than 1.87 of the mean lift force.

3. Comparing the lift force and lateral force to the drag force on each particle at the same Reynolds number and solid fraction, the results show that about 20% to 25% of particles at Re=10 have lift forces more than 10% of drag. However, at Re=200, this number increases to
between 60% to 80%. For the lateral force, approximately 30% to 40% of particles contribute more than 10% of drag at Re=10, whereas between 45% to 50% have lateral forces larger than 10% of drag forces. Neglecting these forces in reduced-order simulations will lead to large errors in resolving particle dynamics.

4. Developing mean correlations for drag, lift, lateral forces, and torque for non-spherical particles based on Reynolds number, void fraction, and particle geometrical factors (incidence angle in this case), will certainly advance the current state-of-the-art for reduced-order simulations. However, this investigation clearly reveals that more advanced sub-scale models are necessary to resolve the large local sub-grid flow driven perturbations imposed on the mean values. The situation is even more challenging for calculating individual particle torques which may not even have the same direction as that indicated by the mean coefficient.

4.8 Acknowledgements

Danesh Tafti would like to acknowledge support from Dr. Mehrdad Shahnam and Dr. William Rogers at the National Energy Technology Laboratory (NETL), Morgantown, WV. The authors acknowledge Advanced Research Computing at Virginia Tech for providing computational resources and technical support that have contributed to the results reported within this paper. URL: http://www.arc.vt.edu.

4.9 Nomenclature

\[ A \] area

\[ d \] distance

\[ D_{eq} \] equal volume sphere diameter
$F$  normalized force
$L$  length
$N$  number of particles
$n$  surface normal
$P, p$  pressure
$Re$  Reynolds number
$t$  time
$T$  torque
$u$  streamwise interstitial velocity
$U$  superficial flow velocity

Greek

$\alpha$  angle describing ellipsoidal particle orientation
$\beta$  angle between the global and local coordinate system
$\gamma$  mean pressure gradient constant
$\lambda$  sensitivity parameter
$\mu$  viscosity
$\rho$  density
$\tau$  shear stress
$\phi$  solid fraction
$\chi$  averaged value
$\psi$  sphericity

Subscripts

$e$  surface element

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Superscripts

* dimensional value

Miscellaneous

\(X, Y, Z\) global Cartesian coordinates

\(X', Y', Z'\) local Cartesian coordinates
### 4.10 Tables

Table 4.1. Geometry parameters and the number of particles for each solid fraction.

<table>
<thead>
<tr>
<th>Geometry parameter</th>
<th>Ellipsoid</th>
</tr>
</thead>
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<tr>
<td>Semi-major</td>
<td>0.921</td>
</tr>
<tr>
<td>Semi-minor</td>
<td>0.368</td>
</tr>
<tr>
<td>Sphericity $\psi$</td>
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</tr>
<tr>
<td>$D_{eq}$</td>
<td>1</td>
</tr>
<tr>
<td>Number of particles $N$</td>
<td></td>
</tr>
<tr>
<td>$\phi = 0.1$</td>
<td>191</td>
</tr>
<tr>
<td>$\phi = 0.2$</td>
<td>382</td>
</tr>
<tr>
<td>$\phi = 0.3$</td>
<td>573</td>
</tr>
<tr>
<td>$\phi = 0.35$</td>
<td>669</td>
</tr>
</tbody>
</table>
Table 4.2 Mean drag force, lift force for ellipsoidal particles in assembly

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<th>Solid fraction</th>
<th>0.1</th>
<th>0.2</th>
<th>0.3</th>
<th>0.35</th>
</tr>
</thead>
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<td>Re</td>
<td>Drag</td>
<td>Lift</td>
<td>Lift/Drag</td>
<td>Drag</td>
</tr>
<tr>
<td>10</td>
<td>4.12</td>
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<td>5.00%</td>
<td>7.92</td>
</tr>
<tr>
<td>50</td>
<td>6.43</td>
<td>-0.68</td>
<td>10.54%</td>
<td>11.80</td>
</tr>
<tr>
<td>100</td>
<td>9.13</td>
<td>-1.32</td>
<td>14.46%</td>
<td>16.00</td>
</tr>
<tr>
<td>200</td>
<td>14.60</td>
<td>-2.88</td>
<td>19.73%</td>
<td>24.90</td>
</tr>
</tbody>
</table>
4.11 Figures

Figure 4.1. (a) Unstructured surface mesh used for representing the immersed boundary. (b) Fluid force on element and the vector from the centroid of the particle to the surface element.
Figure 4.2. Global and local coordinate system. (a) 3D view; (b) x-direction (flow direction) view.
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Figure 4.4. Non-dimensional u-velocity from assembly of ellipsoidal particles at solid fraction of 0.2 and Reynolds number of 100: (a) XZ plane at Y = 0; (b) YZ plane at X = 0.
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Figure 4.9 Total drag force (left column): the blue scatters stand for the total drag force on each particle, and the red scatters are the averaged drag force of particles over every 0.1 radian. Drag force from pressure (right column blue scatter) and viscous shear (right column red scatter) on each particle vs particle incidence angle at solid fraction of 0.35.
Figure 4.10. The mean lift force for ellipsoidal particle at different solid fraction vs Reynolds number.
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Figure 4.12. Total lift force (left column): the blue scatters stand for the total lift force on each particle, and the red scatters are the averaged lift force of particles in every 0.1 radian. The red line is the lift force correlation for isolated single ellipsoidal particle proposed by Zastawny et al [41]. Lift from pressure (right column blue scatter) and viscous shear (right column red scatter) on each particle vs particle incidence angle at solid fraction of 0.1.
Figure 4.13. Total lift force (left column): the blue scatters stand for the total lift force on each particle, and the red scatters are the averaged lift force of particles in every 0.1 radian. The red line is the lift force correlation for isolated single ellipsoidal particle proposed by Zastawny et al [41]. Lift from pressure (right column blue scatter) and viscous shear (right column red scatter) on each particle vs particle incidence angle at solid fraction of 0.35.
Figure 4.14. Probability histogram of ratio between the lift force and drag force on each individual particle.
Figure 4.15. Total lateral force (left column): the blue scatters stand for the total lateral force on each particle, and the red scatters are the averaged lateral force of particles over every 0.1 radian. Lateral force from pressure (right column blue scatter) and viscous shear(right column red scatter) on each particle vs particle incidence angle at solid fraction of 0.1.
Figure 4.16. Total lateral force (left column): the blue scatters stand for the total lateral force on each particle, and the red scatters are the averaged lateral force of particles in every 0.1. Lateral force from pressure (right column blue scatter) and viscous shear (right column red scatter) on each particle vs particle incidence angle at solid fraction of 0.35.
Figure 4.17. Probability histogram of ratio between the lateral force and drag force on each individual particle.
Figure 4.18. Mean torque coefficient variation based on Reynolds number for ellipsoidal particle in assembly at different solid fraction.
Figure 4.19. Torque coefficient at $Z'$ direction on each particle vs particle incidence angle. Each blue scatter represents one particle in assembly, red scatter stands for averaged torque coefficient for particles in every 0.1 radian. The solid red line is the torque coefficient correlation for single isolated ellipsoidal particle proposed by Zastawny et al [41].
Chapter 5

Summary and Conclusion

In this thesis, a framework to study the momentum and heat transfer in the assemblies of particles of any shape is developed. In this framework, the random assembly of particles are generated by the physics engine--PhysX. The particle geometries are resolved using immersed boundary method. The momentum and heat transfer are simulated using particle resolved simulation.

In Chapter 2, ellipsoidal particles with sphericity ($\psi=0.887$) are investigated in a periodic cubic domain to simulate an infinite assembly. Flow through an assembly of spherical particles is tested, and predicted drag forces are compared with previous particle resolved simulation results to validate the current framework. The assembly of ellipsoidal particles is simulated for solid fraction between 0.1 to 0.35 using 191 to 669 particles, respectively, at low to moderate Reynolds numbers ($10\leq \text{Re} \leq 200$). The simulation results show that the drag force of ellipsoidal particles is 15% to 35% larger than equal volume spherical particles. Widely used drag force correlations are evaluated based on the current simulation results. The comparisons show that for ellipsoidal particles over the range of parameters investigated in the present study, the combination of Tenneti et al.’s correlation with Holzer’s single non-spherical particle drag model has the best performance with an average difference of 7.15%.

In Chapter 3, the same ellipsoidal particle is studied in assemblies with a constant heat flux boundary condition applied on the particle surface. Simulation results in the ellipsoidal assembly show that the local velocity and temperature field are significantly affected by the particle orientation. Mean Nusselt numbers for the ellipsoidal assembly are consistently larger than spherical particles when Reynolds number is more than 10, and the difference increases as the Reynolds number
increases. A Nusselt number correlation is proposed based on the simulation data. The proposed correlation is valid in the range $10 \leq Re \leq 50$ for solid fraction of $0 < \phi \leq 0.35$, and $50 < Re \leq 200$ for solid fraction of $0.1 \leq \phi \leq 0.35$.

In Chapter 4, the drag force, secondary forces, and torque are investigated for the ellipsoidal particle. The results show that the mean drag and lift force and torque variations with flow incidence angle on individual particle follow trends similar to that found for isolated particles. However, there are large variations in these quantities under the same conditions of Reynolds number, void fraction, and incidence angle which become more significant as the Reynolds number increases, leading to the conclusion that local flow conditions in the assembly have a large impact on forces and torques experienced by a particle. Comparing the ratio of secondary lift and lateral forces to the drag force on each particle at the same Reynolds number and solid fraction, shows that approximately 80% of particles for lift and 60% for lateral force are within 10% of the drag force at low Reynolds numbers, but a significant number of particles exhibit values greater than 10% (17% for lift and 50% for lateral force) as the Reynolds number increases, leading to the conclusion that neglecting secondary forces can introduce substantial errors. As expected, the mean value of torque coefficient increases with void fraction and decreases with Reynolds number. However, individual particles at the same mean flow conditions show large variations about the mean, even acting in the opposite direction to that indicated by the mean value.

In summary, different computational tools necessary to simulate the momentum and heat transfer in the assembly of particles with any geometric shape is developed. The framework is first tested with spherical particles and then applied to ellipsoidal particles. This framework shows great capability of resolving momentum and heat transfer in fluid-particle system and providing data with
great details. Although only one non-spherical particle shape is studied in current work, this framework is applicable to any particle shape without further development.
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October 20, 2014).


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A. Nusselt number calculation

In chapter 3, Nusselt number is calculated by:

\[ Nu(x) = \frac{1.0}{\bar{T}_s(x) - \bar{T}_m(x)} \]  \hspace{1cm} \text{Equation A.1}

where \( T_s(x) \) and \( \bar{T}_m(x) \) are the non-dimensional surface temperature of the particle and mixed mean temperature of the fluid averaged at each x location. As we discussed in chapter 3, an averaged Nusselt number can be estimated by excluding the thermal developing part in the assembly. This Nusselt number can give us a good estimate of the overall heat transfer between the fluid and the particles. However, this Nusselt number may not be the most representative of the heat transfer at the individual particle level.

A particle based Nusselt number can be calculated by:

\[ Nu_{\text{particle}} = \frac{1.0}{A \int \left( T_s(x) - \bar{T}_m(x) \right) dA} \]  \hspace{1cm} \text{Equation A.2}

where \( T_s(x) \) is the temperature at the immersed surface element of the particle and \( \bar{T}_m(x) \) is the mixed mean temperature, and \( A \) is the surface area of the particle.

Another method to estimate the particle based Nusselt number is:

\[ Nu_{\text{particle}} = \frac{1.0}{A \int T_s \, dA - \bar{T}_m(x)} \]  \hspace{1cm} \text{Equation A.3}

where \( T_s \) is the temperature at the immersed surface element of the particle and \( \bar{T}_m(x) \) is the mixed mean temperature of fluid at the particle central x location.

However, after numerical tests, both Nusselt number defined in Equation and Equation are not suitable in particle assembly. In Equation, because the \( \bar{T}_m(x) \) is calculated over the flow on the
entire YZ plane, when the temperature is highly non-uniform, the $T_s(x)$ can be very close to $\overline{T_m(x)}$ or even smaller than $\overline{T_m(x)}$, the $\frac{1}{A} \int (T_s(x) - \overline{T_m(x)}) \, dA$ can be a very small number (even negative number) which will lead to a non-physical Nusselt number. Similar rule applies to the $\frac{1}{A} \int T_s \, dA - \overline{T_m(x)}$ in Equation.

Figure A.1. Nusselt number calculated based on Equation for ellipsoidal particles at Reynolds number of 10, solid fraction of 0.35. (Negative values and Nusselt number larger than 40 are not plotted)
Figure A.2. Nusselt number calculated based on Equation 5.2 for ellipsoidal particles at Reynolds number of 200, solid fraction of 0.35. (Negative values and Nusselt number larger than 40 are not plotted)
Figure A.3. Nusselt number calculated based on Equation for ellipsoidal particles at Reynolds number of 10, solid fraction of 0.35. (Negative values and Nusselt number larger than 40 are not plotted)
Figure A.4. Nusselt number calculated based on Equation 5.3 for ellipsoidal particles at Reynolds number of 200, solid fraction of 0.35. (Negative values and Nusselt number larger than 40 are not plotted)
B. Additional figures for force variation in assembly of spherical particles

Figure B.5. Total drag force (left column), drag force from pressure (right column blue scatter) and viscous shear (right column red scatter) for spherical particle at solid fraction of 0.1.
Figure B.6. Total drag force (left column), drag force from pressure (right column blue scatter) and viscous shear (right column red scatter) for spherical particle at solid fraction of 0.2.
Figure B.7. Total drag force (left column), drag force from pressure (right column blue scatter) and viscous shear (right column red scatter) for spherical particle at solid fraction of 0.3.
Figure B.8. Total drag force (left column), drag force from pressure (right column blue scatter) and viscous shear (right column red scatter) for spherical particle at solid fraction of 0.35.
C. Additional figures for force and torque variation in assembly of ellipsoidal particles

The following figures are supplementary figures for Chapter 4, based on the simulation results for solid fraction of 0.2 and 0.3.
Figure C.9. Total drag force (left column): the blue scatters stand for the total drag force on each particle, and the red scatters are the averaged drag force of particles over every 0.1 radian. Drag force from pressure (right column blue scatter) and viscous shear (right column red scatter) on each particle vs particle incidence angle at solid fraction of 0.2.
Figure C.10. Total drag force (left column): the blue scatters stand for the total drag force on each particle, and the red scatters are the averaged drag force of particles over every 0.1 radian. Drag force from pressure (right column blue scatter) and viscous shear (right column red scatter) on each particle vs particle incidence angle at solid fraction of 0.3.
Figure C.11. Total lift force (left column): the blue scatters stand for the total lift force on each particle, and the red scatters are the averaged lift force of particles in every 0.1 radian. The red line is the lift force correlation for isolated single ellipsoidal particle proposed by Zastawny et al [41]. Lift from pressure (right column blue scatter) and viscous shear (right column red scatter) on each particle vs particle incidence angle at solid fraction of 0.2.
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Figure C.13. Probability histogram of ratio between the lift force and drag force on each individual particle.
Figure C.14. Total lateral force (left column): the blue scatters stand for the total lateral force on each particle, and the red scatters are the averaged lateral force of particles in every 0.1. Lateral force from pressure (right column blue scatter) and viscous shear (right column red scatter) on each particle vs particle incidence angle at solid fraction of 0.2.
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Figure C.16. Probability histogram of ratio between the lateral force and drag force on each individual particle.
Figure C.17. Torque coefficient at $Z'$ direction on each particle vs particle incidence angle. Each blue scatter represents one particle in assembly, red scatter stands for averaged torque coefficient for particles in every 0.1 radian. The solid red line is the torque coefficient correlation for single isolated ellipsoidal particle proposed by Zastawny et al [41].