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I, **Annette Volk**, hereby submit this original work as part of the requirements for the degree of Master of Science in Mechanical Engineering.

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Quantification of Numerical and Modeling Errors in Simulation of Fluid Flow through a Fixed Particle Bed

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Quantification of Numerical and Modeling Errors in Simulation of Fluid Flow through a Fixed Particle Bed

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Abstract

Detailed description of flow through stationary particle beds is crucial for the design and implementation of municipal water filtration, material extraction systems for nuclear waste and industrial water purification systems. Knowledge of fluid-particle interactions and fluid flow properties through the bed is essential to design, but difficult to determine from experimental investigations. Combined granular-fluid simulation methods such as coupled Computational Fluid Dynamics and Discrete Element Method (CFD-DEM) have been used to bridge this gap in fundamental knowledge. Able to capture details of the small-scale and large-scale interactions that are difficult to study in physical beds, simulation findings have added great understanding to this field. Unfortunately, the reported results are occasionally flawed by a lack of understanding, specifically regarding the magnitude of numerical and modeling errors. Uniform reporting of error, investigations of simulation trend, and proof of mesh-independence have not been performed for granular-fluid simulations.

A standard method of open-source granular-fluid flow simulation known as CFDEM is applied to the simulation of flow through a fixed bed. The Ergun equation is a validated empirical expression used to predict the drag force in fixed bed flow and this prediction is compared directly to simulation results.

A grid-refinement procedure, standard for publication of CFD simulation results, is applied to the CFD-DEM simulations. The solution trend over the refinement range is investigated using the frequency of convergence, convergence types, and the proposed 'offset' method; a comparison of the expected numerical error and actual extrapolated solution error.

An optimal grid size resulting in the least amount of error is investigated by solution trend, drag profile comparison, and the grid-refinement study results. Error is seen to increase in the simulations at both large cell sizes and as the cell size approaches one particle diameter. A new grid-refinement study

application that does not require analytical solution data is shown to be a good predictor of relative error in the grid solutions.

Three drag correlations are applied to model fluid flow through a fixed bed. The Gidaspow drag correlation is an exact representation of the Ergun equation, and shows high accuracy. The Di Felice correlations is a continuous-function representation of expected drag force. The Koch-Hill correlation was developed from LB simulations for fluidization conditions, and is chosen as an example of a poor correlation choice. The grid-refinement study results are able to distinguish the poor performance of the Koch-Hill correlation from the highly accurate Gidaspow and Di-Felice correlations.

The standard grid-refinement study is shown to be applicable to granular-fluid flows, and to produce results that are useful for common modeling choices. Relatively low convergence frequency of the grid-refinement studies is expected to hinder future application by requiring additional grid solutions. This procedure is recommended for all granular-flow simulations since it provides useful information which can prevent common modeling errors that have hampered fluidization research.

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Nomenclature

<u>Symbol</u>	<u>Description</u>
A	Cross-sectional area of fixed bed
C_d	Coefficient of drag
d_p	Particle diameter
D	Bed diameter
D_e	Equivalent channel diameter
e	Coefficient of restitution
e_{21}	Percentage difference between solution values on grids 1 and 2
E_{21}	Percentage difference between solution values on grids 1 and 2 with reference to grid size refinement and order of equations
E_{ext}	Error in extrapolated grid solution
F_{ij}^c	Contact force exerted on particle i by particle j
F_{ik}^{nc}	Non-contact force exerted on particle i by particle j
$f_{g,i}$	Fluid force on particle i
$f_{grav,i}$	Gravitational force on particle i
$F_{n,ij}$	Normal contact force exerted on particle i by particle j
$F_{t,ij}$	Tangential contact force exerted on particle i by particle j
G^*	Equivalent shear modulus
GCI_{21}	Grid Convergence Index indicating the expected numerical error in the finest solution (solution on grid 1)
GCI_R	Initial grid convergence index definition based on a two-grid-refinement study
h	Average CFD cell dimension
H	Bed height
I_i	Moment of inertia of particle i
K	Carman–Kozeny Constant
k_n	Elastic constant for normal contact
k_t	Elastic constant for tangential contact
I_i	Moment of inertia of particle I, for spherical particles: $I_i = \frac{2}{5}m_i R_i^2$
m^*	Average mass of particles in contact
m_i	Mass of particle i
M_{ij}	Contact torque exerted on particle i by particle j
p	Pressure
p	Observed order of accuracy of the solution trend

Δp	Pressure drop over a certain bed / length
R^*	Equivalent radius of particles in contact
r_{21}, r_{32}	Ratio of grid sizes, $r_{21} = h_2/h_1$, $r_{32} = h_3/h_2$
R_i, R_j	Radius of particle i, particle j
R_i	Radius vector of particle i
R_{pf}	Momentum exchange between fluid and particle
R_k	Ratio of change in solutions on progressively refined grids
Re_p	Particle Reynolds number, $Re_p = \frac{\varepsilon \rho_f d_p \mathbf{u}_f - \mathbf{v}_i }{\mu_f}$
S_v	Surface area per unit volume of particles, for spheres $S_v = \frac{6}{d_p}$
Δt_{CFD}	CFD time step
Δt_{DEM}	DEM time step
t_{col}	Collision duration time
t	Time
τ	Fluid phase stress tensor
T_R	Rayleigh time step
U	Superficial fluid velocity, $U = \varepsilon \mathbf{u}_f^* $
$\mathbf{u}_f^*$	Average interstitial fluid velocity
$\mathbf{u}_f$	Interstitial fluid velocity
$\mathbf{u}_s$	Average solids velocity
$\mathbf{v}_i$	Velocity of individual particle i
ΔV_i	Volume of individual CFD cell i
$\mathbb{V}_i$	Volume of individual particle i
$\mathbf{v}_{n,ij}$	Relative normal velocity of particle i to particle j
$\mathbf{v}_{t,ij}$	Relative tangential velocity of particle i to particle j
$\mathbf{w}_i$	Rotational velocity of particle i
x_μ	Particle pair coefficient of friction
Y^*	Equivalent Young's Modulus
Y_i, Y_j	Young's Modulus of particle i, particle j
β	Coefficient of inter-phase momentum transfer
γ_n	Viscoelastic damping coefficient for normal contact
γ_t	Viscoelastic damping coefficient for tangential contact

$\delta_{n,ij}$	Normal overlap between particle i and particle j
$\delta_{t,ij}$	Tangential overlap between particle i and particle j
$\epsilon_{21}, \epsilon_{32}$	Difference between solutions on progressively refined grids
ϵ	Volume fraction occupied by fluid
ζ	Coefficient of restitution function
μ_f	Fluid absolute viscosity
ν_i, ν_j	Poisson ratio of particle i, particle j
ρ_f	Density of fluid
ρ_s	Density of solid (particles)
ϕ_1, ϕ_2, ϕ_3	Solution values on progressively refined grids
ϕ_{ext}	Extrapolated solution value

Chapter 1

Introduction

Granular-fluid flows are commonly used in industrial processes due to the simplicity of their design, high heat transfer rates, ease of control and high efficiency.^{1,2} One particular example of granular-fluid flow is flow through fixed beds.

Fluid travels through fixed particle beds in many practical applications such as filtering, HVAC systems and thermal storage.³ Municipal water is filtered using open-tank bed filters which clarify the water by using a combination of gravel and sand as a filtering device.⁴ Slow sand filtration was recommended by the World Health Organization (WHO) in 1974 as the simplest, most economical and efficient method of water treatment. The WHO noted the widespread use of slow sand filtration in areas ranging from small rural towns to highly industrialized areas.⁵

The success of municipal water treatment plants is dependent on the resulting quality of water and efficiency of the filtering and treating operations. All of these factors rely on adequate knowledge of the fluid behavior as it travels through the filtering substance. If the system is not designed with consideration of the true flow properties, the filtration system is unlikely to produce potable water. Specifically, pressure drop across the filter bed dictates a large portion of the operating cost for filtration as well as the capital required for correctly sized pumps.³

Geankopolis⁴ noted the use of flow through packed beds for fluid to solid ion-exchange processes. Ion-exchange applications include purification, water softening, and extraction of useful materials from nuclear waste.⁶ The hydrodynamics occurring in the bed are essential to the process design and process efficiency. As an example, one of the design criteria specified by Geankopolis was the avoidance of excess pressure drops in the bed as these could deform commonly used gel-resin particles.⁴

Fixed beds are used in a similar manner for adsorption in which unwanted components of a liquid can be separated by a solid adsorbent. Examples of adsorption in which fixed beds are commonly used include removal of sulfur compounds from natural gas, and removal of odor from the air. For these systems to be effective, the substrate must release the adsorbed material to regenerate.⁴ Completed in a cyclic or continuous manner, the regeneration process depends highly on knowledge of fluid-solid interaction.

Fluidized beds, granular conveying flows, and hopper discharge are just a few additional examples of granular flows. Similar to the application of fixed bed flow, the design of these systems relies heavily on knowledge of the interaction between fluid and solid materials. Most interactions between fluid flow and granular particles are difficult, if not impossible, to investigate experimentally due to relatively small-scale interaction phenomena and lack of data acquisition methods for experimental gas-solid flows.

1.1. Motivation

Numerical simulations of granular-fluid interaction have seen recent exponential growth in application frequency. These numerical simulations have shown the potential to capture physical processes and phenomena that cannot be sufficiently determined by experimental data or analytical expressions. Beginning with small-scale validation work, numerical simulations of granular-fluid flow have grown into an increasingly predictive role in academia and industry.^{7,8} However, full verification and validation of the simulation and modeling procedures have not been established. Procedures for uniform reporting of error common in other computational modeling disciplines have not been applied to coupled granular-fluid computations.

The consequences of a lack of adequate verification, validation and uniform reporting procedures are occasionally highlighted in the published literature. To overcome an error generated by lack of knowledge of the required simulation setup, Wang et al.⁹ addressed the claim that a Two-Fluid Model could not adequately model small, cohesive particles, categorized as Geldart type A particles. They found that the Two-Fluid Model was adequate for this scenario when an appropriate value of cell size, much smaller than had previously been examined, was able to accurately capture the physical phenomena. This type of error can slow the progress of simulation development for granular flow applications, and can result in incorrect predictions of granular-fluid flow properties. For granular flow simulations to be dependable for predictive and design applications, adequate verification, validation and uniform reporting procedures must be established.

1.2. Overview of Previous Research

While verification, full validation and uniform reporting procedures have not been established for the modeling and simulation of granular flow, much research has been conducted with these objectives in mind. Verification for this study is defined as ensuring the governing equations are solved using an appropriate method and does not include primary code verification (checking the source solver code for errors).¹⁰ Validation, checking that the correct governing equations are being solved, is attempted in most published papers with excellent examples by Goldschmidt *et al.*¹¹, Li *et al.*⁸, Hoomans *et al.*¹² In 2004, Grace¹³ published a critique of the validation claims by discussing the difference between full validation and practical validation. Grace claimed that published studies performed the required *practical* validation for the situation of interest, but the results of these efforts do not constitute a full validation. While Grace noted the need for full verification and validation, no procedures were proposed to accomplish this task. Preliminary verification and validation of new codes and coupling procedures are still commonly reported, but any expansion of their application range requires additional validation.¹⁴⁻¹⁷

Other researchers have investigated validation of correlations that are essential to simulation of granular fluid flow. Effort has been directed at the establishment and application of various closure relationships commonly used in multi-scale modeling.¹⁸⁻²² Closure relationships such as the correlation for fluid drag force on solid particles have been shown to dictate the accuracy of simulation results.²³ Validity and applicability of these correlations have been investigated for different granular-fluid flows.

For consistent modeling practices, several researchers have attempted to identify an optimal degree of grid-refinement. Optimal grid sizes have been proposed, based on several different criteria such as reduction of total error in a single scenario^{9,24}, accuracy of porosity calculation²⁵ and grid independence of the CFD solution¹⁷. No overriding criteria for optimal grid size have been established, leaving the responsibility of grid development and result validation in the hands of individual researchers.

In 1984, Glicksman²⁶ published a set of non-dimensionalized parameters for fluidized beds which were shown to achieve similitude between industrial and experimental beds. A set of simplified relationships was published by Glicksman *et al.*²⁷ in 1993 for greater flexibility in experimental design. These scaling relationships can be used in simulation development to serve as a basis for non-dimensionalized modeling parameters such as optimal cell size.

1.3. Objectives of this Study

The overarching goal of this study is to establish a fundamental basis for verification and develop uniform reporting procedures for granular-fluid flow computations. This overall objective is addressed via the following tasks:

- 1) Quantify error in simulated solutions for flows through fixed beds using uniform reporting standards
  - a. Analyze CFD-DEM simulation results for flow through a fixed bed using a standard grid-refinement procedure. Compare the results of the grid-refinement study with a known solution to comment on the validity and applicability of the grid-refinement study.
  - b. Use the grid-refinement study results to investigate methods of error reporting that do not require analytical correlations or experimental data for comparison.
- 2) Investigate the solution trend over consecutively refined grids, with emphasis on highlighting regions with asymptotic trends. Identify trends at each of the grid size extremes.
  - a. Search for an optimal grid size within the asymptotic range (if one exists) that exhibits minimal error and can be seen to capture the physics present in the problem.
- 3) Analyze the effect of different drag closures on the simulation results. Examine how uniform error reporting from a grid-refinement study could be useful for quantifying modeling errors.

Chapter 2

Analytical Method

This chapter contains detailed descriptions of analytical expressions for flow through fixed beds and methods of grid-refinement investigation. Section 2.1 presents the development of the theoretical relationship between fluid pressure drop over a fixed bed of particles and the superficial velocity of fluid through the bed. It also describes the assumptions are to simplify the problem, and the resulting series of well-known correlations. The definitive relationship is the Ergun equation, with expression development illustrated in Section 2.1.1. The minimum fluidization velocity, calculated in Section 2.2, is the defined limit of the fixed bed regime as well as the limit of the Ergun equation applicability.

The focus of this chapter shifts to the grid-refinement study procedure in Section 2.3. The development of the grid-refinement study for uniform reporting is given in Section 2.3.1. This is followed by a widely accepted modern grid-refinement method in Section 2.3.2. Finally, an overview of convergence types handled by the grid-refinement study is given in Section 0.

The empirical correlations for fixed-bed pressure drop described in this chapter will be used to analyze simulation result accuracy. The grid-refinement study procedure described in this chapter will also be applied to the simulation results to address the objectives of this study. Results of these applications are included in Chapter 5.

2.1. Pressure Drop Relations for Flow through a Fixed Bed

The expression development for fluid flow pressure drop across a packed bed is given by Rhodes¹. This development features several well-known correlations, and culminates in the Ergun equation.

Darcy was the first to observe that flow through a packed bed resulted in a pressure gradient proportional to the superficial velocity through the bed.²⁸ This observation is fundamental for the development of a series of expressions to define the relationship of pressure gradient to the properties and conditions of the bed.

The relationship of pressure gradient to superficial velocity and bed properties was not immediately evident, and much of the physics occurring in the bed was unknown, prompting researchers to use a unique assumption to relate Darcy's observation to experimental values. They assumed that a fixed bed could be treated as a series of parallel tubes through which fluid was allowed to flow. The laminar flow through a tube had been described by Hagen and Poiseuille as shown in Eq. (2.1):

$$\frac{(-\Delta p)}{H} = \frac{32\mu_f u_f^*}{D_e^2} \quad (2.1)$$

An effective tube diameter and height must be defined to apply this equation to analysis of flow through a fixed bed. The equivalent height was assumed to be proportional to the bed height by an unknown constant. The effective diameter in Eq. (2.2) is based on the hydraulic diameter accounting for the presence of solid particles:

$$D_e = \frac{4 \times \text{flow area}}{\text{wetted perimeter}} = \frac{4 \times \text{flow area}}{\text{wetted surface} / \text{bed height}} \quad (2.2)$$

$$= \frac{4\varepsilon A}{S_v(1 - \varepsilon)AH / H} = \frac{4\varepsilon}{S_v(1 - \varepsilon)}$$

In Eq. (2.2), the flow area is assumed to be constant with bed height, and can be calculated as the void fraction multiplied by the cross sectional area of the bed. The wetted surface, S_v , is a function of the surface area per unit volume of the particles. For perfectly spherical particles, S_v can be calculated directly from the particle diameter, as shown in Eq. (2.3):

$$S_v = \frac{6}{d_p} \quad (2.3)$$

The average interstitial velocity included in Eq. (2.1) is related in a more general form to the superficial velocity as shown in Eq. (2.4). The superficial velocity is synonymous with inlet velocity and empty bed velocity:

$$U = \varepsilon |u_f^*| \quad (2.4)$$

The effective diameter, effective height and superficial velocity definitions are substituted into Eq. (2.1). The result in Eq. (2.5), is known as the Carman-Kozeny Equation:

$$\frac{(-\Delta p)}{H} = K \frac{(1 - \varepsilon)^2}{\varepsilon^3} \mu U S_v^2 \quad (2.5)$$

Where K is known as the Carman-Kozeny constant. Experimental data approximates this constant as 5.

Substitution of the Carman-Kozeny constant value and the expression in Eq. (2.3) for perfectly spherical particles results in the general expression in Eq. (2.6):¹

$$\frac{(-\Delta p)}{H} = 180 \frac{(1 - \varepsilon)^2 \mu_f U}{\varepsilon^3 d_p^2} \quad (2.6)$$

2.1.1. Ergun Equation

In 1949, Ergun and Orning² reviewed previously published correlations and theorized that proper description of the flow required the equation to be expanded to capture two separate behavior regimes. They found viscous forces to be dominant at low velocities and for fine powders. When the bed experienced higher velocities, kinetic effects became dominant. Ergun and Orning² also found that a smooth transition existed between the two regimes, and theorized that a single continuous function could be used this model the transition with upper and lower limits corresponding to the equations for each regime.

They began with the Hagen-Poiseuille Equation, Eq. (2.7), for laminar flow through a tube, and added a term to represent kinetic energy loss:

$$\frac{(-\Delta p)}{H} = \frac{32 \mu_f u_f^*}{D_e^2} + \frac{1}{2} \frac{\rho_f (u_f^*)^2}{D_e} \quad (2.7)$$

Using the equivalent diameter calculation in Eq. (2.2) and the equivalent height assumption, Eq. (2.7) is modified to represent flow through a fixed bed. The result is Eq. (2.8), a combination of the Carman-Kozeny equation and a modified kinetic energy loss term:

$$\frac{(-\Delta p)}{H} = 2C_1 \frac{(1 - \varepsilon)^2}{\varepsilon^3} \mu U S_v^2 + \frac{1}{8} C_2 \frac{1 - \varepsilon}{\varepsilon^3} \rho_f U^2 S_v \quad (2.8)$$

While for laminar flow only, $2C_1 = K = 5$ based the Carman-Kozeny constant, the complete equation requires modified coefficients for an accurate continuous function. Ergun and Orning² proposed values for the constants based on new and published experimental data. The data were chosen to encompass a wide range of solid and fluid properties. The resulting coefficients are combined with the assumption of perfectly spherical particles for the common form of the Ergun Equation, in Eq. (2.9):

$$\frac{(-\Delta p)}{H} = 150 \frac{\mu_f U}{d_p^2} \frac{(1 - \varepsilon)^2}{\varepsilon^3} + 1.75 \frac{\rho_f U^2}{d_p} \frac{1 - \varepsilon}{\varepsilon^3} \quad (2.9)$$

The first term in Eq. (2.9) represents the laminar component (viscous force dominant), and the second term represents the turbulent component (kinetic effects dominant). The plot of pressure drop as a function of superficial velocity in Fig. 2.1 includes three curves corresponding to the total drop in pressure (Eq. (2.9)) as well as the two component contributions contained in Eq. (2.9). The viscous contribution is clearly much smaller than the kinetic energy loss component.

FIG. 2.1: ERGUN EQUATION RESULT AND INDIVIDUAL COMPONENTS

Hence, it is immediately evident that the Carman-Kozeny Equation (laminar term only) is not sufficient to represent the flow properties in this range of void-fraction and superficial velocity. For higher superficial velocities, the kinetic energy loss component accounts for nearly 90% of the pressure loss, as shown in Fig. 2.2.

FIG. 2.2: RELATIVE MAGNITUDE OF VISCOUS AND KINETIC COMPONENTS OF ERGUN EQUATION

The range of validity of the Ergun equation is most efficiently described by the Ergun Reynolds number calculation, Eq. (2.10):

$$Re_{Erg} = \frac{\rho_f U d_p}{\mu_f (1 - \varepsilon)} \quad (2.10)$$

Ergun and Orning² fit their equation to experimental data in the range of $1 < Re_{Erg} < 2400$. However, Allen *et al.*³ found that the Ergun equation consistently over-predicted the pressure drop for Ergun Reynolds Numbers greater than 700 when compared to published experimental results. They noticed that other published correlations deviated from the Ergun equation around this range of Ergun Reynolds number. Based on a wealth of experimental data, Allen *et al.*³ suggested that the original formulation of the Ergun equation should only be applied for smooth spheres below this range of Ergun Reynolds numbers. Montillet²⁹ suggested that a transition to the fully developed turbulent regime, in which the pressure drop is no longer related to the square of the superficial velocity, may account for this divergence of reality from the conditions described by the Ergun equation.

2.2. Minimum Fluidization Velocity

The minimum fluidization velocity is located at the transition between the fixed-bed and fluidized-bed flow regime. Below the minimum fluidization velocity, upward force on the particle mass due to the drag and buoyancy forces is less than the gravitational force on the bed.³⁰ Small particle movements within the bed are likely to occur in this fixed bed regime, but no bulk flow exists. Above the minimum fluidization velocity, bulk movement is common in the bed, and can lead to phenomena such as bed expansion, bubbling and plug flow. Fixed-bed pressure drop correlations such as the Ergun equation require the use of a time-varying void fraction when applied above minimum fluidization velocity.

Minimum fluidization velocity is dependent on bed and fluid properties, and must be calculated for each case. The expression development for minimum fluidization velocity begins with the defined equality of forces acting on the bed, as shown in Eq. (2.11) and Eq. (2.12):

$$\left[\begin{array}{c} \text{Drag} \\ \text{Force} \end{array} \right] = \left[\begin{array}{c} \text{Gravitational} \\ \text{Force} \end{array} \right] - \left[\begin{array}{c} \text{Buoyancy} \\ \text{Force} \end{array} \right] \quad (2.11)$$

$$F_D = (1 - \epsilon)\rho_s g V_{bed} - (1 - \epsilon)\rho_f g V_{bed} \quad (2.12)$$

The drag and gravitational forces are written as averages over the bed volume in Eq. (2.13):

$$\frac{\beta}{\epsilon} [\mathbf{u}_f - \mathbf{v}_i] = (1 - \epsilon)\rho_s g - (1 - \epsilon)\rho_f g \quad (2.13)$$

The expanded expression for drag force will be explained in detail in Section 3.5.5.

The averaged expression in Eq. (2.13) is rearranged to solve for the minimum fluidization velocity. At the minimum fluidization velocity, the solid particles are assumed to be stationary, and the solid velocity is set to zero, resulting in Eq. (2.14),³¹

$$u_{mf} = \frac{\beta}{\varepsilon} (1 - \varepsilon) (\rho_s - \rho_f) g \quad (2.14)$$

The minimum fluidization velocity prediction in Eq. (2.14) is a function of particle properties, fluid properties and the average void fraction. In many desired applications for minimum fluidization velocity prediction, the void fraction at the onset of fluidization is not known. Wen and Yu³² proposed a novel correlation for minimum fluidization velocity in 1966 by noting that the void fraction at incipient fluidization remains fairly constant over a wide range of particles and conditions. This correlation has become widely used as a much simpler prediction mechanism. The Wen and Yu correlation is shown in Eq. (2.15), with the required correlations for Galileo number and particle Reynolds number at minimum fluidization, in Eq. (2.16) and Eq. (2.17) respectively:

$$(N_{Re})_{mf} = \sqrt{(33.7)^2 + 0.408 N_{Ga}} - 33.7 \quad (2.15)$$

$$N_{Ga} = d_p^3 \rho_f (\rho_s - \rho_f) \frac{g}{\mu_f^2} \quad (2.16)$$

$$(N_{Re})_{mf} = \frac{d_p \rho_f u_{mf}}{\mu_f} \quad (2.17)$$

The Wen and Yu correlation in Eq. (2.15) is generally applied for fine particles. Coarse-particle minimum fluidization velocity is more accurately predicted from Eq. (2.18) which was developed by Chitester et al.^{30,33}:

$$(N_{Re})_{mf} = \sqrt{(28.7)^2 + 0.494N_{Ga}} - 28.7 \quad (2.18)$$

2.3. Grid-Refinement Study

A grid-refinement study, also known as a grid convergence study, is a requirement for verification of CFD simulation codes. Assuming the successful completion of basic code verification, grid-refinement studies strive to assess and quantify numerical uncertainty in simulation results.³⁴ Based on the Richardson Extrapolation Method¹⁰, grid-refinement studies are important tools for identifying mesh-independent solutions, determining apparent order of accuracy for numerical schemes and approximating numerical error on a proposed solution grid. The procedure for grid-refinement studies has been developed to obtain uniform reporting of numerical error. The development history of the grid-refinement method is discussed briefly, followed by a well-documented method of grid-refinement based on a recent and commonly cited procedure policy by Celik *et. al.*³⁵

2.3.1. Development of the Grid-Refinement Study

The quantity known as Grid Convergence Index (GCI) was first proposed by Roache in 1994 as a uniform reporting criterion for grid-refinement results.¹⁰ Grid Convergence Index values can be used to compare results of numerical schemes of different orders; one of the many reasons the GCI method has become widely accepted and often required for publication.

The first GCI calculation method proposed by Roache requires solutions on only two grids. Roache began by noting that the quantity often reported in grid-refinement studies was a simple error expression between the two grids in the manner of Eq. (2.19):

$$e_{21} = \frac{(\phi_2 - \phi_1)}{\phi_1} \tag{2.19}$$

With ϕ_1 as the fine-grid solution and ϕ_2 as the coarse-grid solution. This error calculation is based on the assumption that the finer-grid solution is correct. Roache objected to this reporting criterion since it

does not consider the ratio between the grid sizes and the order of the solution. Roache proposed Eq. (2.20) as an alternate method of error reporting:

$$E_1 = \frac{e_{21}}{(r^p - 1)} \quad (2.20)$$

In Eq. (2.20), Roache introduces a correction to the error estimator which considers the refinement rate and numerical solution order. By applying this estimator to several simple examples, Roache found that it did not provide a consistent bound on the error. The corrected operator proved to fluctuate between an optimistic and pessimistic estimate of the actual error for varying numerical solution orders. The error estimated by Eq. (2.20) was expected to be greater than the actual error in only half of the considered scenarios. Therefore, Roache suggested the Grid Convergence Index calculation in Eq. (2.21) as a uniform error estimator:

$$GCI_R = \frac{3|e_{21}|}{(r^p - 1)} \quad (2.21)$$

Roache proposed general reporting of the GCI since the calculation in Eq. (2.21) converts simple error resulting from any numerical scheme to the expected value of the simple error when the grid size is halved ($r=2$) and the calculation is performed with a second order numerical scheme. Roache chose this scenario as the reporting criterion because it results in a conservative estimate of the error.¹⁰

Roache's proposals resulted in a large push for error reporting in CFD. His proposed method became the foundation and motivation for standardizing uniform reporting methods.³⁴ Subsequent researchers modified Roache's methods to develop the error reporting guidelines commonly used today. Roache's use of only two grid solutions in the refinement study was questioned at length, and eventually increased to a minimum of three grid solutions to provide a better overview of solution

trend. The inability of Roache's method to handle oscillating convergence was also addressed by subsequent researchers.

2.3.2. Current Grid-Refinement Study Procedure

The grid-refinement calculations used in this study are based on a recent review of uniform reporting procedures by Celik *et al.*³⁵ Celik et al.'s calculations are developed from Roache's original proposal to include three grid solutions, handle oscillating convergence and calculate the observed order of accuracy. An overview this grid-refinement study procedure is shown in Fig. 2.3.

FIG. 2.3: OVERVIEW OF GRID-REFINEMENT STUDY

Three grid solutions and the ratios between them are required input for the grid-refinement study, as shown on the left hand side of Fig. 2.3. Results of the grid-refinement study include three important quantities: the observed order of accuracy, the extrapolated solution and the grid convergence index (GCI). The calculation of input quantities and the equations used in the grid-refinement study are explained in the following paragraphs.

While structured grids are used for this study, the grid cells are not uniform. A single cell height is required to describe each grid for the study. Volume-averaged cell length³⁵, calculated in Eq. (2.22), is the suggested grid size descriptor for a 3-dimensional grid:

$$h = \left[\frac{1}{N} \sum_{i=1}^N (\Delta V_i) \right]^{1/3} \quad (2.22)$$

In addition to grid size, a single variable of interest must be captured from each grid solution for comparison. The variable (ϕ_n) is an integral quantity critical to the solution or the behavior of the system (the total drag force on the particle bed is the critical quantity in this work for reasons that will be explained later). The difference in this variable for consecutive grid solutions is computed as shown in Eq. (2.23). The fine-grid solution is represented by ϕ_1 , and ϕ_3 represents the coarse-grid solution:

$$\begin{aligned} \epsilon_{21} &= \phi_2 - \phi_1 \\ \epsilon_{32} &= \phi_3 - \phi_2 \end{aligned} \quad (2.23)$$

The ratio between subsequent grid sizes, known as the refinement rate³⁵, is computed from the grids, as shown in Eq. (2.24):

$$r_{21} = \frac{h_2}{h_1} \quad r_{32} = \frac{h_3}{h_2} \quad (2.24)$$

The observed order of the accuracy is determined from the solution trend. Initially, Roache assumed the observed order of accuracy to be the same as the order of the numerical scheme¹⁰, but in reality, the observed order usually does not exactly match the order of the numerical scheme. Therefore, in modern grid-refinement methods, the order of accuracy is calculated from the solution trend. The resulting observed order of accuracy is compared to the numerical scheme order for verification of the software code and numerical solution scheme. In this study, we do not have an

analytical expected order of accuracy of the scheme due to the effect of the coupling procedure on the CFD solution scheme.

The observed order of accuracy of the solution trend³⁵ is determined from iterative solution of Eq. (2.25) and Eq. (2.26):

$$p = \frac{1}{\ln(r_{21})} \left| \ln \left| \frac{\epsilon_{32}}{\epsilon_{21}} \right| + q(p) \right| \quad (2.25)$$

$$q(p) = \ln \left(\frac{r_{21}^{p-s}}{r_{32}^{p-s}} \right), \text{ where } s = 1 \times \text{sign} \left(\frac{\epsilon_{32}}{\epsilon_{21}} \right) \quad (2.26)$$

Each calculated order of convergence value is checked to be non-zero and non-infinite. A zero or infinite observed order of accuracy value indicates a poorly designed grid-refinement study that cannot correctly analyze the solution trend.

The observed order of accuracy is used to calculate the extrapolated solution and the grid convergence index. The extrapolated solution value³⁵, calculated using Eq. (2.27), is the expected value of the mesh independent simulation based on the solution trend with decreasing cell size across the three grid solutions:

$$\phi_{ext} = \frac{\phi_1(r_{21})^p - \phi_2}{(r_{21})^p - 1} \quad (2.27)$$

For the present study, the extrapolated solution error is calculated in Eq. (2.28) to quantify how close the solution trend converges towards the known Ergun equation value. The error, E_{ext} , between the converged and Ergun equation value is due to modeling errors with respect to the correlation or unrecognized numerical errors:

$$E_{ext} = \left| \frac{\phi_{ext} - \phi_{Ergun}}{\phi_{Ergun}} \right| \quad (2.28)$$

The final result of the grid-refinement study is the Grid Convergence Index (GCI), calculated using Eq. (2.29):

$$GCI_{21} = \frac{1.25|\epsilon_{21}|}{(r_{21})^p - 1} \quad (2.29)$$

GCI is the expected numerical error in the finest grid solution based on the solution trend.³⁵ The GCI does not account for modeling errors with respect to the Ergun equation correlation as only the solution trend with decreasing cell size is analyzed.³⁴

2.3.3. Convergence Categories

In addition to the grid-refinement study, each set of three grid solutions is sorted into a general convergence category based on the general solution trend. This convergence category is a general description of the solution trend³⁴ based on the value of R_k shown in Eq. (2.30):

$$R_k = \frac{\epsilon_{21}}{\epsilon_{32}} \quad (2.30)$$

The accuracy of error estimates from the grid-refinement study is partially based on the convergence category of the solution trend. Converging trends feature more accurate error estimates than diverging trends.

The ideal case resulting in the best error estimates is a positive convergence criteria value, R_k , that is less than one. An R_k value in this range is an indication of monotonic convergence, and all three grids can be assumed to reside in the asymptotic range. Negative values of the convergence criteria with magnitude less than one indicate oscillatory convergence. In oscillatory convergence, the solutions

converge towards the solution, but the grid size or numerical scheme prevent an ideal monotonic solution trend.³⁴

If the magnitude of R_k is greater than one, the solution trend is diverging. Positive values of the convergence criteria in this range indicate monotonic divergence, while negative values indicate oscillatory divergence.³⁴ An example of the solution trend in each convergence category is shown in Fig. 2.4. The solution convergence or divergence occurs as the cell size is reduced from the large cell sizes on the right to the smaller cell sizes to the left in each plot.

FIG. 2.4: SOLUTION TREND CONVERGENCE CATEGORIES
 (A) $R_k = -0.5$ (B) $R_k = -2$ (C) $R_k = 0.2$, (D) $R_k = 2$

Chapter 3

Numerical Method

This chapter contains an overview of the mathematical formulation of the problem with the numerical schemes and implementations used to determine the numerical solution. First, a description of numerical implementations for the analysis of multiple scales of fluidized bed behavior is given in Section 3.1. The advantages and disadvantages of each implementation are discussed at length, and the choice of a coupled CFD-DEM solution method is justified.

Section 3.2 is a discussion of the advantages associated with the open-source software utilized in this study. The complete open-source software set of OpenFOAM, LIGGGHTS, CFDEM Coupler and Paraview is described.

Sections 3.3 through 3.5 outline the separate components of the numerical implementation. Section 3.3 begins with the computational fluid dynamics (CFD) part which approximates the Navier-Stokes Equations for the fluid domain. The Navier-Stokes Equations are modified from their original form to include particle porosity in the mass balance and particle-fluid interaction forces in the conservation of momentum. The complex dependence of the solution on the grid size is discussed.

The discrete element method (DEM) equations for particle-momentum conservation based on Newton's second law are contained in Section 3.4. The choice of the soft-sphere model over the hard-sphere model is justified in Section 3.4.1, and the soft-sphere model equations are outlined in Section 3.4.2. Correct soft-sphere model implementation requires an adequately small time step, and multiple correlations for critical time step are explained and compared in Section 3.4.3. The use of a reduced stiffness value to increase computational efficiency is proposed in Section 3.4.4.

The CFD and DEM calculations are linked by the CFDEM coupling, as detailed in Section 3.5. An unresolved coupling method is determined to be more applicable to this study than a resolved method in Section 3.5.1. The open source software description in Section 3.5.2 is followed by an overview of the coupling procedure in Section 3.5.3. Special attention is given to the choice of porosity calculation method in Section 3.5.4, as this can be crucial to accurate calculation of particle-fluid contact forces. Finally, a selection of drag models is defined for use in the coupling regime, and the correlation values are compared across a wide range of void fraction and superficial velocity values in Section 3.5.5.

3.1. Multi-Scale Modeling of Fluidized Beds

Fluidized beds contain physics in a large range of scales that are vital to the bed behavior. Industrial sized beds can feature meter-wide flow structures that are crucial to their implementation and design. In the same bed, particle-scale interactions on the order of millimeters can be important to the bed behavior. The largest flow structures in the bed usually depend directly on the particle-scale structures and their interactions.²² These large-scale variations cannot be represented efficiently or effectively in a single simulation, so closure relationships have been developed to represent the details of the small-scale interactions for use in larger scale simulations. An overview of the simulations scales is shown in Fig. 3.1.³⁶ Each simulation scale is discussed in detail, beginning with the finest scale.

FIG. 3.1: OVERVIEW OF SIMULATION SCALES AND CLOSURE RELATIONSHIP DEVELOPMENT³⁶

The finest-scale simulations address scales smaller than particle scale, and are grouped as Direct Numerical Simulations (DNS). Requiring eight or more cells per particle gap, these simulations commonly use the Lattice-Boltzmann Method (LBM), a finite-difference scheme that solves the Boltzmann Equation.³⁶ The LBM formulation models the particle-fluid boundaries with a sticking condition, assuring a simple and accurate boundary condition implementation.³⁶ Traditional CFD methods can be used to model this scale of interaction^{37,38}, but the boundary condition implementation is more complicated and often less accurate. Typical LB simulations model fluids flowing through a fixed array of particles since modeling particle movement is computationally expensive and particle contacts

cannot be handled by this method.^{18,23,36,38} Direct numerical simulations with fluid-particle interaction forces based directly on first principles³⁹ do not require closure equations or empirical coefficients as the smallest-scale structures and interactions are modeled directly.^{38,40} The only primary modeling error present in the LB simulations is the inability to capture the true diameter of the particles. Due to the nature of the boundary condition implementation, an effective diameter - differing from the input diameter - must be determined.²³ This effective diameter is reported as the particle diameter, and can be easily determined from the simulated terminal velocity of a single particle.³⁶ DNS simulations are too computationally expensive to model systems of the scale of lab experiments,³⁹ as the maximum particle number remains of the order of thousands of particles.⁴¹ LB simulations are typically used to develop drag correlations, since the drag force on each particle can be numerically calculated exactly from these simulation results.^{42,43} These drag correlations are employed in larger-scale simulations to represent the influence of small-scale interactions.

One scale larger than DNS, the Discrete Particle Model (DPM) is typically implemented as a coupling of CFD and DEM.³⁶ Rather than resolving each particle individually, DPM features cells that can contain between 100 and 1000 particles. As an Eulerian-Lagrangian coupling, DPM can track individual particle movements and estimate the interstitial fluid properties. Details of the particle-particle and particle-wall collisions are modeled with resultant forces calculated directly. Particle-fluid interaction forces are estimated from a specified drag correlation.³⁹ The DPM has been used to study potential causes of heterogeneous flow such as the amount of energy dissipated during collisions,⁴⁴ non-linearity of fluid-particle drag with gas fraction,^{45,46} and anisotropy in velocity distribution due to particle clustering.²² Since it can handle beds of the order of millions of particles, DPM is used to model systems large enough to be compared with lab experiments. However, for larger systems DPM is computationally expensive, especially for fine powders.⁴⁷ In a few cases this work load can be reduced by using simplifying assumptions, such as the use of a 1D fluid profile, and a 3D particle configuration to

model plug flow in a horizontal pipe by Tsuji *et al.*⁴⁸ Unfortunately, this type of simplifying assumption is typically not valid.

Two-Fluid Models (TFM) operate at the largest of the commonly used simulation scales. First completed by Davidson in 1961,⁴⁰ Two-Fluid Models are most commonly used for multi-phase flows. A TFM is able to model beds of the order of 100 million to 1 billion particles, and therefore can be used to simulate small industrial-scale systems. The TFM treats granular material as a continuum that is allowed to interpenetrate the fluid phase, resulting in an Eulerian-Eulerian model. The properties of the solid phase continuum are based on closure relations for effective solids viscosity and pressure. A more detailed description of the solid phase can be implemented based on a solid stress tensor, which uses granular temperature to represent the physical properties of the particles.⁴⁴ The solid's continuum properties are difficult to determine from experimentation, but are relatively simple to calculate from DPM simulations.^{22,49} The requirement for, and heavy dependence on, closure relationships is a major detriment to TFM because these constitutive equations cannot be applied generally and must be individually developed for each granular system.^{37,47} Even when applied with detailed and accurate closure relations, the general omission of collision friction in TFM can lead to under-prediction of solids shear viscosity.²² While Two-Fluid Models can be applied to larger-scale systems, more general and descriptive constitutive relations for the solid phase are required for consistent, accurate and more widespread implementation.

A few larger-scale methods have been developed but are not widely accepted. Van der Hoef *et al.*³⁶ developed a Bubble Model in 2004 to model the largest scale interactions in industrial-sized fluidized beds. Based on the Discrete Bubble Model for gas-liquid systems, this method treats bubbles as discrete objects. As a new but promising method, the Bubble Model has not been expanded for additional implementation. In 2007, Tsuji⁴⁰ published results for a one-dimensional calculation operating at the same scale as the bubble model. The calculation was used to model pneumatic conveying by treating

the particles as a single mass with an overall drag coefficient defining fluid force on the total particle mass cross sectional area. While these larger-scale simulation methods are interesting, they can only be used for very specific applications and, therefore, are not widely employed.

3.2. Open-Source Software Advantage

Open-source software is used for modeling and simulation in this work. Four main open-source codes are required, and the calculation procedures implemented in these codes are described in length. The main codes reference other open-source software in their implementation for correct processing. Only the main codes are described as they are critical to the implementation and customization of the numerical calculations.

The first open-source code is OpenFOAM in which the computational fluid dynamics equations are numerically solved as described in Section 3.3. Section 3.4 provides a description of the required DEM calculations which are handled by a code known as LIGGGHTS. LIGGGHTS stands for ‘LAMMPS Improved for General Granular and Granular Heat Transfer Simulations’ where LAMMPS was the original granular dynamics code developed by Sandia National Laboratories, and stands for ‘Large Atomic and Molecular Massively Parallel Simulator.’⁵⁰ The Open Source CFDEM coupling regime handles the data analysis and information exchange between OpenFOAM and LIGGGHTS. The full coupling procedure is described in Section 3.5. After the CFD-DEM calculation is complete, the results are visualized in Paraview. Paraview is included in the CFDEM coupling software, and is used to post-process most of the results presented in Chapter 5.

A fully open-source implementation was chosen for this study due to several distinct advantages. The most widely recognized advantage of open-source codes over commercial codes is the price. Commercial software for computational simulation is often very expensive and this expense is multiplied many times over when the simulation must be run on multiple cores. While cost was a consideration in the choice of codes for this study, it was not the deciding factor for open-source implementation.

An advantage of all open-source software is the ability to view and modify the source code, which cannot be accessed in commercial codes. This allows the user to have complete knowledge of the calculations occurring during the simulation. User modification of the source code can be used to increase computational efficiency for certain applications or to modify numerical schemes for better accuracy, stability or convergence rate. Modified functions such as drag correlation equations, contact models for DEM particles, additional inter-particle forces or turbulence models in CFD calculations can be added to the source code and tested. This allows a level of customization, not available in commercial codes, which has great advantages for skilled users.

A unique advantage of the CFDEM coupling regime is full parallelization of the calculation.⁵¹ Full parallelization can provide computationally efficient calculations of large domains with large numbers of particles.¹⁴ The coupling procedure can be implemented on distributed memory machines where each processor handles its own memory. A skillful user can use distributed memory implementation to increase computational efficiency by distributing the processes (in this case, particle numbers and fluid domain) equally over the processors. Goniva *et al.*⁵⁰ expounded on the distributed-memory implementation as a way to model industrial-sized systems. This advantage is not available in most commercial codes that require shared-memory machines.⁵¹

Kloss *et al.*¹⁵ demonstrated the ability of the CFDEM coupling to perform both resolved and unresolved coupling methods, allowing greater flexibility in implementation within a single code. These coupling methods with their advantages and disadvantages will be described in detail in Section 3.5.1. As a demonstration of the power of the cooperation between CFDEM Project's users and development team, Smuts *et al.*¹⁷ highlighted the four-way coupling method employed in the CFDEM implementation that is not available yet in some commercial code releases.

3.3. Computational Fluid Dynamics (CFD)

Equations for the conservation of mass and momentum of the fluid phase are numerically approximated by the Computational Fluid Dynamics (CFD) solver. The Navier-Stokes Equations and the mass conservation equation are modified for a granular-fluid flow. The CFD solver does not resolve individual particles, but the particle effect is approximated by a void fraction and particle-fluid interaction term that are determined by the coupling procedure. The CFD solver accepts these quantities, and applies them in the governing equations.

3.3.1. Conservation Equations

The CFD equations are simplified for the assumed incompressible flow considered in the present system. The first equation is the continuity equation for the conservation of mass¹⁵ in Eq. (3.1):

$$\frac{\partial \varepsilon}{\partial t} + \nabla \cdot (\varepsilon \mathbf{u}_f) = 0 \quad (3.1)$$

The second fundamental equation is the incompressible Navier-Stokes equation for conservation of momentum [Eq. (3.2)]. The particle effect is included in the void fraction correction of the velocity and the particle-fluid interaction force, $\mathbf{R}_{pf}$.¹⁵

$$\frac{\partial (\varepsilon \mathbf{u}_f)}{\partial t} + \nabla \cdot (\varepsilon \mathbf{u}_f \mathbf{u}_f) = -\varepsilon \nabla \frac{p}{\rho_f} - \mathbf{R}_{pf} + \nabla \cdot \boldsymbol{\tau} \quad (3.2)$$

The expected maximum Reynolds number (Re) value based on the column diameter is around 13,000. Turbulence is expected at this value of Re, but according to Alobaid and Eppe,⁵² turbulence effects will not be significant in flows containing solids concentrations greater than 0.001. Link *et al.*⁵³ also justified the neglect of turbulence by stating that turbulence effects, such as velocity fluctuations, are significantly smaller than the allowed cell size. Link *et al.*⁵³ also noted that particles reduce the

turbulent effects without being affected by the turbulent velocity fluctuations. Nevertheless, turbulent effects are included in this study via the realizable k- ϵ model. A commonly used model realizable k- ϵ is only moderately computationally expensive and has been shown to be a good representation of kinetic effects.⁵⁴ While the turbulence is expected to have very little effect on the solution, it is included for correctness since the success of this study depends on accurate modeling of the physical conditions. The assumption of negligible turbulence was seen to result in only 0.56% change in simulation results with the percent change at each velocity value included in Appendix B.

3.3.2. Implementation

The CFD solution procedure is implemented within OpenFOAM using the pisoFoam module.⁵⁵ First proposed by Issa,⁵⁶ the PISO solution method is employed to approximate the equations for conservation of mass and conservation of momentum.

3.3.3. Importance of Grid Size

In computational modeling applications such as CFD, attainment of consistently valid, accurate simulation results requires the solution to be mesh independent. Mesh independence is the achievement of a constant solution across several grids of decreasing cell size. The validity of CFD-DEM results is similarly dependent on mesh independence, but this quality is difficult to achieve.¹⁷

For all grid-based computational modeling, the cell size must be sufficiently small to capture the governing physics in the system. The system behavior may contain complicated velocity and pressure profiles due to turbulence or intricate geometry that must be captured by the simulation. In granular flows, a bubbling effect is often crucial to the system behavior.⁵⁷ The cell size must be significantly smaller than the bubble size for the simulation to accurately represent and correctly handle the resultant inhomogeneous void fraction profile. If the cell size is too large, unphysical smoothing of the pressure, velocity and void fraction profiles can result in neglect of the true particle interaction with the

fluid.¹⁷ Many granular flow phenomena are not well understood, so the neglect of these physics could be easily overlooked. An oversight of this kind can result in reporting of incorrect results and incorrect predicted behavior in granular systems, and may delay or derail future research in the area.

While large cell sizes may lead to error, cells that are too small can also cause serious errors in CFD-DEM results. The theorized presence of a critical minimum length is one of the reasons that mesh independence is expected to be so difficult to achieve in coupled particle-fluid simulations. The unresolved CFD-DEM method is based on the continuum assumption for the particle-fluid mixture, and allows the simulation to estimate the interaction forces without resolving the small-scale interactions. The mixture is assumed to be a continuum in each separate cell but this may not be a good assumption when the cell size is not sufficiently larger than the particle size.¹⁷ In small cells, the majority of the cell may be filled with a single particle rather than the expected fluid-particle mixture. The use of inappropriately small cells can cause large discontinuities in the void fraction profile, and lead to physically incorrect results.

Many authors have attempted to determine an optimal cell size which results in the highest accuracy simulation results. Each reported optimal size is based on a unique justification. In each case, the optimal size is non-dimensionalized as the ratio of average cell dimension to particle diameter for general application and comparison.

Wang *et al.*⁹ and Sturm *et al.*²⁵ recommend a cell size to particle diameter ratio of 3. Wang *et al.*⁹ analyzed fluidized bed expansion with the use of a Two-Fluid Model. Of the four grid solutions they obtained, only the finest resulted in good quantitative agreement for the bed expansion. They theorized that the grid size to particle ratio of 3 was sufficient to resolve the particle clustering formations in the bed.⁹ While Sturm *et al.*²⁵ recommended the same optimal ratio, their recommendation is based on a

study by Gotz²⁵ in 2006 where a cell size to particle diameter ratio of 3 was shown to be optimal for porosity calculation accuracy.

Muller *et al.*²⁴ compared three different grid solutions with experimental results. Rather than using a standard grid-refinement procedure, they refined each grid using an independent method which resulted in elongated rectangular cells. Their grid solution under-predicted the void fraction profile when the minimum cell dimension was 1.5 particle diameters in the in-plane direction. However the under-prediction did not occur when the flow-direction cell dimension was reduced to 2 particle diameters. Muller *et al.*²⁴ recommended a cell size between 3 and 4 particle diameters for their application since this size range consistently led to solutions with good quantitative comparison to experimental data. Similarly, Link⁵⁸ compared solutions on a fine grid of 1 particle diameter cell length with a coarse grid of 4 particle diameter cell length. His coupling procedure represented each particle as a porous cube to expand the particle effect over several grid cells and prevent local discontinuities in the void fraction profile. Comparison of the two grid solutions revealed only small differences, so he recommended the coarse grid size of 4 particle diameters.

Finally, Smuts, Deglon, and Meyer¹⁷ recommended a ratio of 4.2 particle diameters per cell length as a compromise between accurately capturing the physics in the CFD calculation and satisfying the continuum assumption for the unresolved coupling method. They completed a grid-refinement study of the CFD calculation by neglecting the particle presence and determined the solution at this grid size to be mesh-independent. The complete CFD-DEM solution on this recommended grid was compared to the solution on a coarse grid with cell dimensions of 5.6 particle diameters. Significant differences between the solutions led Smuts *et al.*¹⁷ to recommend the finer cell size of 4.2 particle diameters.

While many methods have been used to determine the optimal cell size to particle diameter ratio, none of these methods have shown a complete justification of the recommended value.

Comparing between several grid solutions is an important step in determining the optimal ratio, but may not be sufficient. The full solution trend with changing grid size must be understood since the grid size is expected to be limited below some critical maximum and above some critical minimum cell size. Comparing only two consistently refined grids does not sufficiently eliminate the possibility of violating one of these critical size limits. In the present study, several new methods of determining the optimal grid size to particle diameter ratio are introduced and compared. The theoretical basis behind each method is discussed in detail.

3.4. Discrete Element Method (DEM)

The discrete element method (DEM) is used to individually track particles using a force balance based on Newton's second law of motion. This method was first applied to granular materials by Cundall and Strack in 1979.⁵⁹ This section describes the available DEM models, an overview of the chosen soft-sphere model equations, and considerations for the time step and spring constant values.

3.4.1. Hard Sphere vs. Soft Sphere Model

Two major model types are available for DEM. Cundall and Strack⁵⁹ introduced the soft-sphere model in their revolutionary work on granular DEM in 1979. In the soft-sphere model, particles are allowed to overlap slightly while retaining their spherical shape.⁶⁰ Campbell and Brennen⁶¹ introduced the hard-sphere model in 1985 which assumes non-overlapping stiff particles.

The soft-sphere model is driven by time. Collisions are detected and resultant forces calculated at the end of each time step. In contrast, the hard-sphere model is collision driven, and the simulation is treated as a series of individually resolved, instantaneous collisions.⁴⁴ While the soft-sphere model is applicable to all types of granular simulations, the hard-sphere model is only applicable for dilute systems. Resolving each collision as a discrete event, the hard-sphere model cannot handle multi-particle contacts such as those occurring during packing and settling.⁶⁰ For rapid and dilute granular flows, hard-sphere models are far more computationally efficient than soft-sphere models due to the small time step required for the soft-sphere model. In the soft sphere model, each time step must be significantly smaller than the particle collision duration⁶² to prevent unphysical increases in total system kinetic energy as well as infeasible particle overlap. The hard-sphere model does not suffer from this limitation since the simulated time between each calculation is dictated by the time between collisions.

To increase computational efficiency in the soft-sphere model, the particle stiffness value is often decreased; increasing the collision duration and the critical time step.⁴⁴ In some studies, multiple

simulations with different particle stiffness values are compared, and they show minimal effect of the reduced stiffness.⁴⁷ Since this stiffness reduction is common, other studies have simply assumed that this unphysical value will have no effect on the results, e.g. Silbert *et al.*⁶² who stated they chose a stiffness value that they “believe captures the general behavior of intermediate-to-high- k [stiffness] systems.”

The hard-sphere model is capable of using the actual particle stiffness in its calculations without repercussions on the computational efficiency. However, the hard sphere model has a unique limitation of its own. Termed ‘inelastic collapse’ by McNamara and Young⁶³ in 1992, the hard-sphere model was shown to result in an un-physically large decrease in system kinetic energy when modeling a particle number density above a critical value or a coefficient of restitution below a critical value. Inelastic collapse occurs when the hard sphere model attempts to model long-term or multiple-particle contacts. Instead of recognizing the constant contacts between particles, the system predicts an infinite number of collisions in a finite amount of time.

The final item of consideration in the choice between hard-sphere and soft-sphere models is the implementation of long-range inter-particle forces. Long-range forces such as electrostatic forces are important factors in certain types of granular flows.⁶⁴ The soft-sphere model is able to implement these forces, while the hard-sphere model is not.⁶⁰

The soft-sphere model was chosen for the present application due to the high particle number density present in the simulated system. Modeling of fixed beds requires resolution of a lattice of constant contacts between particles, and this is likely to cause inelastic collapse in the hard-sphere method.⁶³ For a feasible time step in the soft-sphere model, the particle stiffness value must be reduced; this would be readily incorporated in the hard sphere model.

3.4.2. Soft-Sphere Model Equations

The DEM solution procedure is based on Newton's second law and the conservation of momentum. The mass is inherently conserved since each particle is individually tracked. At some boundaries, particles are allowed to leave the simulation domain, but the transfer of their mass to outside the domain is accounted for in the mass balance.

The conservation of momentum contains linear and angular components. The linear-momentum conservation equation calculates the change in linear momentum of each individual particle based on the total forces applied. The linear-momentum equation⁶⁴ is shown in Eq. (3.3), with terms individually labeled in Eq. (3.4):

$$m_i \frac{d\mathbf{v}_i}{dt} = \sum_j \mathbf{F}_{ij}^c + \sum_k \mathbf{F}_{ik}^{nc} + \mathbf{f}_{grav,i} + \mathbf{f}_{g,i} \quad (3.3)$$

$$\begin{aligned} \left[\begin{array}{c} \text{Time Rate of Change in} \\ \text{Momentum} \end{array} \right] &= \left[\begin{array}{c} \text{Sum of Contact} \\ \text{Forces} \end{array} \right] + \left[\begin{array}{c} \text{Sum of Non-Contacting} \\ \text{Forces} \end{array} \right] \\ &+ \left[\begin{array}{c} \text{Gravitational} \\ \text{Force} \end{array} \right] + \left[\begin{array}{c} \text{Particle-Fluid} \\ \text{Interaction Force} \end{array} \right] \end{aligned} \quad (3.4)$$

Each set of forces is handled separately in the DEM procedure. The contact forces are based on a chosen particle-contact model. Non-contact forces are neglected in the present study since the particles are not charged, and are large enough that electrostatic forces do not affect the behavior of the bed. The gravitational force is applied at the center of the particle, and is based on the particle's mass. The particle-fluid interaction force is calculated by the coupling regime for each particle based on values from the CFD and DEM calculations.

The conservation of angular momentum is written similarly with the change in angular momentum of each particle equated to the sum of moments of forces acting on the particle. The

moment of forces, calculated for a single particle (i) in Eq. (3.5), depends only on the tangential contacting force. As shown in Eq. (3.6), the moment is summed⁶⁴ over all of the contacting particles (j):

$$\mathbf{M}_{ij} = \mathbf{R}_i \times \mathbf{F}_{t,ij} \quad (3.5)$$

$$I_i \frac{d\mathbf{w}_i}{dt} = \sum_j \mathbf{M}_{ij} \quad (3.6)$$

To calculate changes in linear and angular momentum, the DEM solver identifies particle contacts and determines the resultant forces. Two particles are determined to be in contact if the distance between their centers is less than the sum of their radii. While this overlap check is a simple distance calculation, large numbers of particles can make this procedure very inefficient as each particle must be checked with N-1 particles for possible contact. The concept of neighbor lists was developed to reduce this computational burden. Neighbor lists are developed for each individual particle, and contain a list of the particles within a certain range of the particle of interest. The included particles are likely to currently be in contact or to soon establish contact with the particle of interest. Neighbor lists can be maintained for several iterations and contain all of the possible contact pairs.⁶⁵ The neighbor-list method reduces the number of possible particles that must be analyzed at each time step for positive contact.

The Hertz Model⁶⁶ is chosen for calculating the resultant contact force. The resultant force calculation in Eq. (3.7) consists of a normal component and a tangential component:

$$\mathbf{F}_{ij}^c = [k_n \delta_{n,ij} - \gamma_n \mathbf{v}_{n,ij}] + [k_t \delta_{t,ij} - \gamma_t \mathbf{v}_{t,ij}] \quad (3.7)$$

The Hertz model equation consists of four coefficients multiplied by the normal and tangential overlaps and relative velocities to determine the total force vector. The model coefficients are based on

particle properties including radius, Young's Modulus, Poisson ratio, mass, and coefficient of restitution. The coefficients are also functions of the normal and tangential overlap, and must be calculated for each contact at each time step. An overview of these equations is given in Table 3.1 in Eq.(3.8) to (3.15).⁶⁶

TABLE 3.1: HERTZ CONTACT MODEL COEFFICIENT EQUATIONS

Normal Overlap	δ_n	(3.8)
Elastic Constant for Normal Contact	$k_n = \frac{4}{3}Y^*\sqrt{R^*\delta_n}$	(3.9)
Viscoelastic Damping Coefficient for Normal Contact	$\gamma_n = -2\sqrt{\frac{5}{6}}\zeta\sqrt{S_n m^*} \geq 0$	(3.10)
Elastic Constant for Tangential Contact	$k_t = 8G^*\sqrt{R^*\delta_n}$	(3.11)
Viscoelastic Damping Coefficient for Tangential Contact	$\gamma_t = -2\sqrt{\frac{5}{6}}\zeta\sqrt{S_t m^*} \geq 0$	(3.12)
Overlap Function for Normal Contact	$S_n = 2Y^*\sqrt{R^*\delta_n}$	(3.13)
Overlap Function for Tangential Contact	$S_t = 8G^*\sqrt{R^*\delta_n}$	(3.14)
Coefficient of Restitution Function	$\zeta = \frac{\ln(e)}{\sqrt{(\ln e)^2 + \pi^2}}$	(3.15)

Coefficient calculations for the Hertz Model contact force contain equivalent particle properties. These properties are averaged over the contacting particle pair and must be calculated individually for each contact. The averaging methods given in Table 3.2, Eq. (3.16) to Eq. (3.19), do not affect the results of this study, since all of the particle properties are identical.

TABLE 3.2: EQUIVALENT PARTICLE PROPERTY EXPRESSIONS

Equivalent Mass of Particles (i, j) in Contact	$\frac{1}{m^*} = \frac{1}{m_i} + \frac{1}{m_j}$	(3.16)
Equivalent Radius of Particles (i, j) in Contact	$\frac{1}{R^*} = \frac{1}{R_i} + \frac{1}{R_j}$	(3.17)
Equivalent Young's Modulus of Particles (i, j) in Contact	$\frac{1}{Y^*} = \frac{(1 - \nu_i^2)}{Y_i} + \frac{(1 - \nu_j^2)}{Y_j}$	(3.18)
Equivalent Shear Modulus of Particles (i, j) in Contact	$\frac{1}{G^*} = \frac{2(2 - \nu_i)(1 + \nu_i)}{Y_i} + \frac{2(2 - \nu_j)(1 + \nu_j)}{Y_j}$	(3.19)

The tangential component is truncated in order to satisfy the Coulomb Friction Law in Eq. (3.20) which states that the tangential force component cannot exceed the normal force component multiplied by the coefficient of friction. If the two sides of Eq. (3.20) are equal, the particle pair is sliding relative to each other⁶⁷:

$$|\mathbf{F}_{t,ij}| \leq x_\mu |\mathbf{F}_{n,ij}| \quad (3.20)$$

The collision forces for all contacts occurring during a single time step are calculated, and the resulting forces are employed in the conservation of momentum in the subsequent time step.

3.4.3. Time Step Value

The soft-sphere model is time-driven, this allows for multiple contacts to occur during a single time step. The time step is a critical value, and the DEM solution must be shown to be time step-independent. Several researchers have attempted to determine the critical value of the time step based on particle and system properties. The theoretical foundations of three unique methods to calculate the critical time step are discussed and compared.

O'Sullivan and Bray⁶⁸ recommended a critical time step calculation based on the maximum frequency of the contact force equation. This maximum frequency, and therefore, the critical time step, is based on the square root of the ratio of minimum particle mass to the maximum stiffness value, as shown in Eq. (3.21):

$$\Delta t_{DEM} \leq 0.17 \sqrt{m_{min}/k_{max}} \quad (3.21)$$

Both minimum particle mass and maximum stiffness value in Eq. (3.21) are subject to change at each time step. The minimum particle mass may change due to changes in the individual particles

involved in collisions. The maximum stiffness is a function of the overlap which is expected to change at each time step for each collision. While this method may be used to check the critical time step using the simulation results, it is not able to predict the required time step.

Silbert *et al.*⁶² developed an expression for the critical DEM time step based on the collision time. They theorized that 50 time steps were necessary to correctly model a collision. The time step in Eq. (3.22) is based on the estimated collision duration calculation in Eq. (3.23):

$$\Delta t_{DEM} \sim \frac{t_{col}}{50} \quad (3.22)$$

$$\text{where } t_{col} = \pi \left(\frac{2k_n}{m} - \frac{\gamma_n^2}{4} \right)^{-1/2} \quad (3.23)$$

Silbert's method suffers the same detriment as O'Sullivan and Bray's method in which the calculated critical time step is based on time and collision-dependent properties. The elastic and viscoelastic coefficients are functions of the particle overlap, which is time dependent. For most applications, the particle mass is time dependent since it is determined from the particle with the greatest mass involved in a collision at the time of interest.

Finally, Ren *et al.*⁶⁹ theorized that, since only two particles can be considered in each contact, the numerical time step must be small enough compared to the force transmission that the effects of a pair collision cannot spread beyond the involved particles and the fluid that surrounds them. The resulting critical value of time step can be determined from the Rayleigh force transmission wave speed as shown in the Rayleigh time step calculation in Eq. (3.24):

$$T_R = \frac{1}{2} \pi d_p \left(\frac{\rho_p}{G^*} \right)^{1/2} (0.1631v + 0.8766)^{-1} \quad (3.24)$$

The Rayleigh time step [Eq. (3.24)] is a function of constant particle properties. The particles involved in collisions may change with time, but particle properties which minimize the Rayleigh time step (such as the maximum Poisson ratio ν) are used in this equation. Equation (3.24) does not require the use of simulation results, and provides a conservative estimate of the Rayleigh time step.

The standard practice for DEM time step determination is described by Ren *et al.*⁶⁹ In Eq. (3.25), a conservative estimate of 20% of the Rayleigh time step is used to ensure that the true physical force transmission is only between neighboring particles:

$$\Delta t_{DEM} \sim 0.2 T_R \quad (3.25)$$

At time steps greater than the recommended value from Eq. (3.25), the simulation may mistake force transmissions between multiple particles as only affecting the collision pair, and can result in inaccurate results and instability in the numerical scheme.

3.4.4. Spring Constant Value

One disadvantage of the soft-sphere model is the frequent inability to use physically correct values for the spring constant. Large values of the spring constant require very small time steps, and greatly reduce the computational efficiency, occasionally preventing even the ability to simulate. Therefore, it has become standard practice to use smaller values of the stiffness, since usually this reduced value does not affect the simulation results.⁴⁷ The spring constant value must be large enough to avoid large amounts of penetration.⁶² Tsuji, Kawaguchi and Tanaka⁴⁷ investigated a spring constant value reduction by comparing results from different stiffness values. They found very little difference in the simulation results as the fluid-particle interaction force was the main determinant of bed behavior.

The spring constant value is expected to have very minimal effect in the regime of flow through a packed bed. The particle Young's modulus value is therefore reduced several orders of magnitude. The critical time step is a factor of one over the square root of the shear modulus, and therefore the Young's modulus. As an example, a reduction in Young's Modulus value by a factor of 100 will increase the allowable time step by a factor of 10.

3.5. CFDEM Coupling

The CFDEM Coupling post-processes the results obtained from the DEM and CFD solvers to calculate the interaction forces between fluid and solid phases. This section describes the available coupling types, code implementations, and a detailed coupling procedure for the chosen open-source platform.⁷⁰ Details of the equations within the coupling are discussed in detail, with emphasis on the porosity calculation and drag correlations.

3.5.1. Coupling Types

Two types of CFDEM couplings can be used to link the fluid-dynamics and discrete-element methods. Resolved methods are used when a small number of considered particles have a large diameter with respect to the system geometry. Grids for the resolved method are designed such that particles completely cover multiple cells. For an accurate calculation, Hager *et al.*¹⁴ found that at least 8 cells were required per particle diameter, while Kloss *et al.*¹⁵ recommend 10 cells per particle diameter. This fine grid is required to accurately represent the particles and this approach can be combined with other available methods to resolve the particle boundaries. Examples of such methods include immersed boundary method, dynamic mesh refinement, and a VOF-type treatment of cells partially filled with solid.¹⁴ The group of cells located within an individual particle is treated as a fictitious domain, ensuring the velocity is constant for the entire particle.

The need for an initially fine mesh with the possibility of additional refinement indicates a very computationally expensive simulation. Therefore, resolved calculations can only be used for very small-particle systems of the order of hundreds of particles.¹⁴

The other available coupling method, known as the unresolved method, is used when the geometry is relatively large compared to the particles. The particles are treated by averaging over the cell in which they are located. The only information passed by the coupling regime is the porosity and

velocity functions of the solids, and the fluid-particle interaction force can be calculated from these quantities. The cell size is larger than the particle diameter, and this allows for modeling of much larger systems.

The unresolved method is chosen for the present research since it is much more computationally efficient and can handle systems with the order of millions of particles. This is essential as the fixed bed setup of interest is expected to contain around 20,000 particles, and multiple simulations must be run for this system in a reasonable computational time.

3.5.2. Implementation

The coupling procedure is implemented using the open-source CFDEM Coupling. CFDEM Coupling assumes the use of LIGGGHTS and OpenFOAM, as the DEM and CFD solver, respectively. The porosity calculation methods and drag correlations discussed in this section are implemented in the base source code of the CFDEM Coupling regime.

3.5.3. Coupling Procedure

An overview of the coupling procedure is shown in Fig. 3.2. The calculation procedure begins with the DEM calculation in LIGGGHTS (Step 1). A single time step is computed to initialize the particles which in many cases have been previously modeled in a pure DEM simulation. The coupling regime calculates the porosity and average particle velocity in each cell (Step 2). This information is used with the specified initial fluid velocity and pressure field to calculate the fluid-particle momentum exchange based on the chosen drag closure equation (Step 3). The resulting momentum exchange term along with the porosity field is passed to the CFD calculation in OpenFOAM. The updated velocity and pressure fields are calculated in OpenFOAM based on this information (Step 4). Multiple iterations are run in OpenFOAM until the residuals are below the required values for convergence. The momentum

exchange term passed to the CFD calculation is decomposed into forces on individual particles based on the initialized CFD fields, cell porosity and particle velocity functions (Step 5).⁵⁰

FIG. 3.2: COUPLING PROCEDURE FOR CFDEM

The next DEM calculation (Step 1) accounts for the momentum-exchange term in the particle momentum-conservation equations. Due to a significantly smaller critical time step, 50-100 DEM time steps are typically completed for each CFD time step.¹⁷ The fluid-particle interaction force on each particle is kept constant throughout the DEM calculation set of time steps. The ratio of DEM to CFD time steps must be large enough to be computationally efficient since the maximum allowable DEM time steps can be several orders smaller than CFD time steps. The time step ratio must also be small enough that a constant momentum exchange over the set of DEM time steps is an appropriate assumption, and does not affect the accuracy of the solution.

3.5.4. Porosity Calculation

The fluid-solid interaction is determined from the porosity and velocity fields. Velocity fields are relatively simple to calculate from the results of each (DEM, CFD) calculation; these are passed on to the coupling regime. The porosity field is more difficult to calculate in an accurate, reproducible manner. Since the bed behavior is highly sensitive to the porosity field, this calculation is very important to the overall accuracy and physical correctness of the simulation results. We examined several different porosity calculation methods to determine the optimal method for the present application; these are described next.

The simplest porosity calculation method is known as the Centered Volume Fraction (CVF) Method. In this method, each individual particle is located only by its center, and the entire particle is considered to be located in the cell where the center lies. This is very computationally efficient, but leads to high uncertainty in the porosity field.⁷¹ Kloss *et al.*¹⁵ noted that this method leads to poor results when the particle size and cell size are similar. Using the CVF method, they observed large variations in the calculated porosity field where none were physically present, and termed this phenomenon ‘artificial inhomogeneity.’

The Offset Method has been used to increase the accuracy of the CVF Method. In the offset method, each computational cell is spatially offset a certain number of times, and the porosity is calculated for each offset position using the CVF method. Sturm *et al.*²⁵ used the offset method combined with a contour-aligned method to accurately calculate porosity near cylinder walls. Alobaid and Epple⁵² showed that the offset method reduced the variation in calculated porosity on a grid with predefined porosity. However, the offset method requires porosity calculations for 27 displacements of each grid cell, and this is very computationally expensive.

Another proposed porosity calculation for increased accuracy is the Divided Volume Fraction (DVF) Method. In the DVF method, each particle is represented by several marker points instead of a single center point. The cell location of each of the n marker points is credited with a solids volume of $1/n$ of the particle volume. This method has been shown to be significantly more accurate, but less computationally efficient than the CVF method. Kloss *et al.*¹⁵ noted that errors in the porosity calculation were still present in this method when the cell size and particle size were similar.

A more recent method known as Artificial Particle Inflation (API)¹⁵ has been used for porosity calculation with great success. For API, each particle is represented as a large porous particle¹⁵ or a large porous cube.⁵³ This method is more numerically stable than the other porosity calculation methods,¹⁵ and reduces the variation in the porosity field as the cell size is reduced towards the particle size.⁵³ This type of calculation can also be done using a separate particle and fluid grid. Porosity calculations are completed on the relatively large particle grid, and the results are transferred to a fluid grid, independent of particle size, by means of averaging and linear interpolation of gradients.⁷¹ While it occasionally produces better results than more traditional methods, the API method does not produce entirely accurate results in most cases. Algorithms that can be used to reduce this inaccuracy are very computationally expensive.⁵⁸

The Divided Volume Fraction (DVF) Method is chosen for use in the present application. The DVF method is highly accurate, except for some reported errors when the cell size and particle size are similar. The DVF method is also computationally efficient compared to the more intensive methods. This porosity calculation method was also chosen because it did not rely on unphysical characteristics, such as solid particles treated as larger porous particles, and maintained conservation of particle mass within the coupling regime.

3.5.5. Drag-Closure Equations

Drag-closure equations are used to estimate the force exchange between solid particles and interstitial fluid. Physically, this force exchange occurs individually for each particle in the boundary layer of fluid surrounding the particle. This physical exchange is not directly modeled in unresolved CFDEM since the fluid cells are significantly larger than the particles. Estimates of the force exchange are labeled as drag-closure equations, and can be developed from several different sources including experimental data, theoretical correlations and lattice Boltzmann (LB) simulations.

Drag correlations are developed from certain physical conditions, but most correlations attempt to cover all possible granular fluid interaction scenarios. These generalizations can have varying degrees of success, as not all granular fluid interactions are well understood, and proposed drag correlations are occasionally missing important physics. Over-expansion of the correlation applicability can lead to large under- and over-prediction of the drag force as well as unphysical degrees of inhomogeneity. There is no recommended 'optimal' drag correlation due to different approaches in drag-correlation formulation and application.

While many drag correlations are available, only three are considered in the present work. These commonly used drag correlations were chosen to represent the variation in available models. The Koch-Hill Drag equation^{18,19} was developed from LB simulations covering a wide range of physical conditions. The Gidaspow drag correlation³¹ is a combination of the Ergun Equation and Wen and Yu equations. The DiFelice drag correlation⁷² is an empirical relation for a larger range of void fraction, particle Reynolds number and flow regime.²¹

To simplify comparison, the drag correlations are written in terms of the coefficient of inter-phase momentum transfer in Eq. (3.26) as suggested by Ku, Li, and Lovas:²¹

$$f_{g,i} = \frac{\mathbb{V}_i \beta}{(1 - \varepsilon)} [\mathbf{u}_f - \mathbf{v}_i] \quad (3.26)$$

The inter-phase momentum transfer coefficient, β , is calculated from the chosen drag correlation. In each correlation, this coefficient is a function of fluid properties, particle properties, relative velocity and void fraction.

The Koch-Hill drag correlation^{18,19} was introduced in 2001, and is based on LB simulations covering a wide range of Reynolds number. It is proposed as a single drag correlation for all granular-fluid interaction scenarios. Ku, Li and Lovas²¹ noted that Koch and Hill's published LB simulations do not include the range of void fractions typically found in fluidized beds. The momentum transfer coefficient calculation for the Koch-Hill method is shown in Eq. (3.27):

$$\beta = \frac{18\mu_f \varepsilon^2 (1 - \varepsilon)}{d_p^2} \left[F_0(\varepsilon) + \frac{1}{2} F_3(\varepsilon) Re_p \right] \quad (3.27)$$

The inter-phase momentum transfer coefficient, β , calculation contains two functions, F_0 and F_3 , that are expanded in Eq. (3.28). The first of these functions, F_0 , contains a step change at the void fraction value of 0.6:

$$F_0 = \begin{cases} \frac{1 + 3\sqrt{\frac{1-\varepsilon}{2}} + \frac{135}{64}(1-\varepsilon)\ln(1-\varepsilon) + 16.14(1-\varepsilon)}{1 + 0.681(1-\varepsilon) - 8.48(1-\varepsilon)^2 + 8.16(1-\varepsilon)^3} & \text{for } (\varepsilon > 0.6) \\ \frac{10(1-\varepsilon)}{\varepsilon^3} & \text{for } (\varepsilon \leq 0.6) \end{cases} \quad (3.28)$$

$$F_3 = 0.0673 + 0.212(1 - \varepsilon) + \frac{0.0232}{\varepsilon^5}$$

The Gidaspow drag correlation³¹ is a combination of the Ergun Equation and the Wen and Yu Equations. In the momentum transfer coefficient calculation of Eq. (3.29), these two drag correlations remain separate, and the step change between them is located at a void fraction value of 0.8 (80%). The Ergun equation is used to describe the fluid-particle interaction of any granular mixture with void fraction less than 0.8 (80%); the Wen and Yu correlation is only used for very dilute flows with particle volume fraction less than or equal to 0.2 (20%):

$$\beta = \begin{cases} \frac{150(1-\varepsilon)^2\mu_f}{\varepsilon^2 d_p^2} + \frac{1.75(1-\varepsilon)\rho_f}{\varepsilon d_p} |\mathbf{u}_f - \mathbf{v}_i| & \text{for } (\varepsilon < 0.8) \\ 3/4 C_d \frac{(1-\varepsilon)\rho_f}{d_p} |\mathbf{u}_f - \mathbf{v}_i| \varepsilon^{-2.65} & \text{for } (\varepsilon \geq 0.8) \end{cases} \quad (3.29)$$

The Wen and Yu correlation in Eq. (3.29) contains the drag coefficient (C_d) which is calculated using Eq. (3.30). While Eq. (3.30) appears to contain a step change, the lower particle Reynolds number function converges towards the higher particle Reynolds number coefficient value, and no large discontinuities are present at the transition. This is not the case for the step change in Eq. (3.29):

$$C_d = \begin{cases} \frac{24}{Re_p} (1 + 0.15 Re_p^{0.687}) & \text{for } (Re_p < 1000) \\ 0.44 & \text{for } (Re_p \geq 1000) \end{cases} \quad (3.30)$$

The Gidaspow drag correlation³¹ is very commonly used. However, the presence of a discontinuity in the correlation implementation was theorized to cause errors.⁷³ This predicted error was the motivation for development of the Di-Felice drag correlation.⁷²

The Di-Felice drag correlation⁷² is based on a similar combination of empirical correlations, but does not contain a discontinuity in the correlation implementation. The correlation shown in Eq. (3.31) can be implemented across all values of void fraction as a continuous function:

$$\beta = 3/4 C_d \frac{(1 - \varepsilon)\varepsilon\rho_f}{d_p} |\mathbf{u}_f - \mathbf{v}_i| \varepsilon^{-\chi} \quad (3.31)$$

Similar to the Wen and Yu correlation, the Di Felice correlation⁷² is based on a separate expression for coefficient of drag, as shown in Eq. (3.32):

$$C_d = \left(0.63 + \frac{4.8}{\sqrt{Re_p}} \right)^2 \quad (3.32)$$

The model of Di Felice was founded on the assumption that drag on a particle when surrounded by other particles is equivalent to the drag on the same particle in the absence of other particles multiplied by some voidage function. DiFelice⁷² calculated the exponent of the voidage function in Eq. (3.33) based on fitting this assumption to experimental data:

$$\chi = 3.7 - 0.65 \exp \left[\frac{-(1.5 - \log_{10}(Re_p))^2}{2} \right] \quad (3.33)$$

The application of the Koch-Hill, Gidaspow and Di Felice models will be analyzed in the present study by comparison of the simulation results obtained with each of the drag correlations.

3.5.5.1. Analytical Comparison

Before applying these correlations in a simulation, they are analytically compared by their calculated drag profiles at the expected fixed-bed void-fraction value. The drag-correlation results are

also compared to the expected Ergun Equation value using calculated error (direction and magnitude) across the domain of possible void fraction and superficial velocity combinations.

The drag correlation results are compared in Fig. 3.3 for the expected void fraction value in the simulated bed, ($\varepsilon \sim 0.43$).

FIG. 3.3: DRAG CORRELATION RESULTS FOR SIMULATION VOID FRACTION

At this value of void fraction, the Gidaspow Model is the exact Ergun Equation result. As seen in Fig. 3.3, both Di Felice and Koch-Hill Models under-predict the Ergun Equation result at this void fraction. While the void fraction value used in this calculation is the average for the bed, the actual calculated void fraction values in the bed will vary. Therefore, the drag correlations are analyzed over a larger range of void fraction. A contour plot of the absolute error for the Di-Felice Model is shown in Fig. 3.4.

FIG. 3.4: ABSOLUTE ERROR BETWEEN DI-FELICE AND GIDASPOW DRAG CORRELATION VALUES

From Fig. 3.4, we see that the best agreement is located at combinations of low void fraction and low superficial velocity. Higher values of void fraction and superficial velocity result in errors of up to 70%. Very low values of these quantities result in similarly large error. The actual error is plotted in Fig. 3.5 where large under-predictions at high values of voidage and superficial velocity can be seen. Error at low voidage and low superficial velocity values is due to large over-prediction of the Ergun results for drag force.

FIG. 3.5: ERROR BETWEEN DI-FELICE AND GIDASPOW DRAG CORRELATION VALUES

The same analysis is conducted for the Koch-Hill drag correlation, and results in the absolute error contour plot shown in Fig. 3.6. The lowest error values are located at high void fraction and low superficial velocity values. The error in this region is low relative to the error in the remainder of the analyzed area, but remains 20% larger than the Ergun equation predicted total drag force.

FIG. 3.6: ABSOLUTE ERROR BETWEEN KOCH-HILL AND GIDASPOW DRAG CORRELATION VALUES

The Koch-Hill drag correlation leads to higher overall error than that obtained with the De-Felice Drag correlation. In the plot of actual error in Fig. 3.7, the Koch-Hill drag correlation consistently underpredicts the Gidaspow drag correlation by up to 70%.

FIG. 3.7: ERROR BETWEEN KOCH-HILL AND GIDASPOW DRAG CORRELATION VALUES

The Di Felice and Koch-Hill drag correlations differ significantly from the Gidaspow drag correlation. Since the Gidaspow correlation is an exact representation of the Ergun equation, we expect simulation results using the Gidaspow correlation to closely match the Ergun equation results. Results from application of the Di Felice and Koch-Hill correlations are expected to exhibit large errors when compared to the Ergun equation values.

Chapter 4

Simulation Method

The simulation is designed to model a commonly used, experimental-sized fixed bed. Emphasis in the simulation design is placed on accuracy and computational efficiency. Description of the simulation method includes specifications regarding the geometry in Section 4.1, computational grid design in Section 4.2, the initialization process in Section 4.3, input properties in Sections 4.4 through 4.6 and output processing of the simulation data in Section 4.7. Each step of the developed method is justified based on published methods and relationships to physical processes. The assumptions at each step are noted and explained. Input property assumptions are analyzed during the setup process to determine their corresponding effect on the results. Possible effects of the general assumptions outlined in this section are discussed at length in Chapter 5.

4.1. Geometry and Boundary Conditions

A 0.1542m (6 inch) diameter column is partially packed with 6mm diameter Airsoft pellets. The height of the bed is determined from the number of initialized particles, and requirements for the bed height are discussed in Section 4.5. In the radial direction, the column features a column diameter to particle diameter ratio of 25.4.

The boundary conditions are independently specified for the CFD and DEM solvers. The coupling routine does not require any boundary conditions. An overview of the column geometry and corresponding boundary names are given in Fig. 4.1. Each implemented boundary condition is justified directly from the corresponding experimental setup.

FIG. 4.1: OVERVIEW OF COLUMN GEOMETRY WITH (A) PHYSICAL CONDITIONS AND (B) BOUNDARY NAMES

In the physical test stand, the inlet consists of a perforated plate stationed above a large chamber to produce a nearly uniform flow. The inlet velocity boundary condition is assumed to be uniform flow with non-zero magnitude only in the axial direction. The inlet velocity magnitude is deliberately changed with time, but the pressure boundary condition at the inlet is kept constant as a

zero gradient condition. The inlet void fraction is specified as a fixed value of 1 to indicate that no granular material is entering with the inlet flow. The perforated plate at the inlet is selected in the experimental design so that particles cannot pass through the perforations. In the DEM procedure, particles interact with the inlet in the same manner as they interact with the solid walls.

The outlet boundary is located at a significant distance above the top of the bed, and is treated as an atmospheric outlet. The outlet pressure is specified as atmospheric, while the velocity profile is modeled as fully developed by a zero gradient condition tangent to the boundary. Since the outlet is located far above the bed, the void fraction is set at a constant value of 1. The DEM solver allows particles to pass through this boundary, but due to the nature of expected bed behavior, no particles are expected to contact this boundary. Hence, the total number of particles throughout the simulation is expected to remain constant.

Finally, the cylinder walls are modeled with a slip condition in the CFD solver. Wall effects are not expected to be large and have been neglected in the theoretical correlations against which the simulation results will be compared. Neglecting wall effects in the CFD simulation allows the grid-refinement considerations to neglect the change in resolution of the wall area as the grids are refined. The pressure and void fraction boundary conditions are set as zero gradient to model a solid (non-porous) boundary. The DEM solver resolves continuously occurring collisions between particles and the cylinder walls. The wall is treated in each collision as exhibiting particle solid properties, infinite mass and zero momentum. Within the fixed bed, the lattice of particle contacts is expected to include the walls at many points.

4.2. Computational Grid Design

The initial grid generation and proposed refinement procedure are crucial to the success of a grid-refinement study. The cylinder column is divided into nearly uniform mesh cells which can be easily modified to consistently refine the grid.

Typically in CFD applications, the cells will be of a variety of sizes that can all be modified in a consistent manner. Refined areas of the grid are modified in the same manner as the rest of the grid to analyze how each mesh can capture smaller effects such as wall effects and turbulence. For packed-bed flow, the cell size to particle diameter ratio is crucial, so ideally the cells will all be identical in size. This desired condition prevents the use of an axisymmetric cylindrical grid which prescribes cells around the axis of the column to be significantly smaller than in the rest of the domain. This size differential would likely cause issues with the porosity calculation, and could preclude good grid-refinement study results.

Instead, the domain is divided into separate sections which are individually meshed. A square is inscribed on the inside of the bottom of the cylinder. The square center is located at the axis (center) of the column, and the size of the square is significantly smaller than the column radius as shown in Fig. 4.2. Each vertex of the square is connected to a point on the cylinder projected from the center axis point as a primary grid line.

FIG. 4.2: AREA DIVISION OF COLUMN BOTTOM FOR FACE-MAPPED GRID

The mesh is generated on this surface by treating the face as five separate areas and mapping the grid within each area. Fig. 4.3 is an example of the separated areas with highlighted primary grid lines for clarity.

FIG. 4.3: GRID GENERATION ON BOTTOM COLUMN FACE BY MAPPING

The mapped grid is extruded in constant segments to the remainder of the column as shown in Fig. 4.4.

FIG. 4.4: EXTENSION OF GRID WITH EQUAL SPACING ALONG COLUMN HEIGHT

To cover the range of cell size to particle diameter ratio that is expected to provide accurate results, 13 total grid-refinement levels are created using the blockMesh feature included in the OpenFOAM installation. The mapped bottom cylinder face, extruded grid along the height and averaged cell size to particle diameter ratio (R) for each grid are shown in Fig. 4.5. The average cell height for each grid is calculated from Eq. (2.22) in Section 2.3.2.

(c) $R = 1.60$

(d) $R = 1.74$

(e) $R = 1.89$

(f) $R = 1.94$

(g) $R = 2.14$

(h) $R = 2.38$

FIG. 4.5: COMPLETE SET OF 13 GRIDS RANGING FROM (A) FINEST TO (M) COARSEST

4.3. Initialization

Initialization in the physical experiment consists of pouring the granular material into the column and allowing the particles to settle. Typical experimental columns are over a meter tall, and the granular material is dropped a significant distance. The high kinetic energy developed from this drop will cause some particles to bounce for a non-trivial amount of time as they dissipate energy. Interactions between the particles and interstitial air will also occur in this period. A computationally expensive simulation would be required to model the significant physical settling time during which particles experience non-trivial interactions with interstitial air. Fortunately, several assumptions and generalizations can be made about this settling process.

The air effects during settling are not expected to have a significant influence on the final configuration of the packed bed. Additionally, the particle configuration resulting from a large drop in an experiment is assumed to be similar to the configuration resulting from a short drop for the simulated mono-sized particle mixture. The application of these assumptions permits a pure DEM simulation of the settling process.

Particles are initially placed throughout the bed using an overlap checking feature which prevents unphysical overlap of the particles as they are added. Due to the nature of the overlap check, the particles cannot all be added at once, but must be added over time. All of the particles are added within the first 1000 time steps (0.02 seconds) and then allowed to settle. The DEM simulation is run with a larger time step than the CFDEM simulation since the particle interactions with time do not have a high

required accuracy. The simulation models a total physical time of 2 seconds in which the kinetic energy profile shown in Fig. 4.6 converges to achieve near-zero values. The kinetic energy in the bed at the end of the settling is of the order of 10^{-9} Joules.

FIG. 4.6: KINETIC ENERGY PROFILE DURING SETTLING

The settled particle bed in Fig. 4.7 is the initial DEM condition for the CFDDEM simulations. The particles are completely settled in the bed, and a contact lattice is fully developed at this time with 42,266 total particle contacts (5 average contacts per particle). An additional random settled particle bed was simulated and the results compared to the initialization process used in this work. The total drag profile with superficial velocity varied from the results in this study by only 0.57%. Therefore, the results are not highly dependent on the initialization procedure.

FIG. 4.7: SETTLED PARTICLE BED

The fluid phase is initialized with zero velocity and constant pressure throughout the domain to simulate the start-up process used in a typical fixed-bed experiment. No momentum exchange occurs between the particles and fluid for the first calculation based on these initial conditions.

After the calculation is initialized, the inlet velocity is immediately increased to the first value of interest. The transition from zero velocity to a finite velocity in a single time step causes the spike in pressure drop over the bed shown in Fig. 4.8. Residence time at the first value of velocity is extended to allow this initial pressure variation to converge to the steady-state value.

FIG. 4.8: INITIAL SPIKE IN PRESSURE PROFILE DUE TO VELOCITY STEP-CHANGE

4.4. Velocity Profile

The inlet velocity profile with time is designed to reproduce the common experimental procedure of incrementally increasing the superficial velocity. At each value of interest, the velocity is held constant for a prescribed residence time, to allow the pressure drop over the bed and total drag force on the particles to reach steady state. Experimental residence time can be 1 minute or greater, but the required simulated time is significantly less due to complete control of superficial velocity and quick data acquisition. The simulation also produces step changes in the inlet velocity with no velocity overshoot, which is impossible experimentally.

An initial velocity profile was chosen with a residence time of 0.1 seconds at each velocity increment. Analysis of the pressure drop over the bed and total drag force with time revealed that a reduced residence time was sufficient for pressure profile convergence at all of the velocity increments except for the foremost velocity increment. The final velocity profile shown in Fig. 4.9 features a 0.1 second residence time for the first velocity increment and a 0.04 second residence time for the remaining incremental velocity changes. The superficial velocity is varied between 0.1 and 1.1 m/s in 0.1 m/s increments. This covers a wide range of flow through the fixed bed with Ergun Reynolds numbers ranging from 64 to 703.

FIG. 4.9: INLET VELOCITY PROFILE WITH TIME

In Fig. 4.10, pressure drop over the bed is plotted with time for the entire simulation. The pressure drop over the bed is found to reach a steady-state value within the allowed residence time for each of the velocity increments examined.

FIG. 4.10: PRESSURE DROP OVER PARTICLE BED WITH TIME

The pressure drop profile in Fig. 4.10 appears to reach steady state significantly faster than the prescribed residence time for most of the investigated velocity values. While decreasing the residence

time may seem advantageous, magnification of the pressure drop trend with time in Fig. 4.11 reveals the motivation for retaining the full residence time.

FIG. 4.11: PRESSURE DROP OVER PARTICLE BED WITH TIME: DETAILED

Each velocity step-change causes an initial pressure drop overshoot immediately followed by a nearly steady-state value. While the pressure drop remains nearly constant during the remainder of the residence time, small variations are present. These small variations are due to small particle movements as the bed adjusts to the imposed drag forces. These small variations affect the steady-state pressure-drop values for current and subsequent velocity increments. Particle beds have been known to adjust slightly to reduce resistance to the flow. This is an important physical process that is captured by the simulation.

The drag force trend in Fig. 4.12 is a similar trend of quick convergence followed by small variations during the residence time. Comparison of the detailed drag trend in Fig. 4.13 with the corresponding pressure trend in Fig. 4.11 demonstrates the expected correlation between pressure and drag variations.

FIG. 4.12: TOTAL DRAG FORCE WITH TIME

FIG. 4.13: TOTAL DRAG FORCE WITH TIME: DETAILED

The proposed velocity profile is based on the desired flow regime of flow through a fixed bed. Any bulk movement, expansion, or bubbling in the bed would indicate that a fluidized-bed regime has been reached and the analytical correlations used in this study are no longer valid. The Ergun equation solution is calculated from a constant void fraction value, and this is not physically correct for modeling bed expansion. Several methods are used to check for fluidization conditions, including particle contact

analysis, visual analysis of bed, and pressure profile analysis. These methods require a fluidized bed for comparison, so the velocity profile is expanded from a maximum value of 1.1 m/s to a new maximum value of 1.5 m/s. This new maximum superficial velocity is near than the predicted minimum fluidization velocity of 1.52 m/s from Eq. (2.18) in Section 2.2.

The trend of particle contacts in the bed is examined in a manner similar to that used by Kafui *et al.*⁷³ Upon initialization (e.g. particle settling) each particle is in contact with an average of 5 other particles, indicating a well-developed contact lattice in a settled bed. The average number of contacts per particle at the end of each velocity increment residence time is shown in Fig. 4.14. At the end of the proposed velocity trend (max velocity of 1.1 m/s), each particle is in contact with approximately 4.8 other particles. At the end of the new velocity profile (maximum velocity of 1.5 m/s), each particle is in contact with approximately 3.5 other particles.

FIG. 4.14: AVERAGE CONTACTS PER PARTICLE WITH INCREASING SUPERFICIAL VELOCITY

The trend of particle contacts shown in Fig. 4.14 has a large reduction in particle contacts beginning at a superficial velocity of 1.2 m/s. There is negligible change in the average number of particle contacts for superficial velocities less than this critical value. The maximum superficial velocity

investigated in this study (1.1 m/s) appears to be in the fixed-bed regime, based on the consistency of the average number of particle contacts.

The bed expansion can also be examined qualitatively. A snapshot of the bed with a superficial velocity of 1.1 m/s is compared to the bed with a superficial velocity of 1.5 m/s in Fig. 4.15. The lighter colored particles indicate higher applied drag force.

FIG. 4.15: COMPARISON OF BED BEHAVIOR WITH SUPERFICIAL VELOCITY 1.1 M/S AND 1.5 M/S

The bed with superficial velocity value of 1.5 m/s in Fig. 4.15 is clearly expanded as expected from the trend of large-particle behavior published by Geldart and Cranfield.⁷⁴ This expansion is not present at a superficial velocity of 1.1 m/s. In Fig. 4.16, the bed at the maximum proposed velocity of 1.1 m/s is compared to the original packed bed to demonstrate that expansion due to bulk movement has not taken place in the bed.

FIG. 4.16: COMPARISON OF BED BEHAVIOR WITH SUPERFICIAL VELOCITY 1.1 m/s, AND INITIALLY SETTLED

The final check for fluidization is a qualitative comparison of the drag force profile (or alternately, pressure profile) with time. The total drag force with time is plotted in Fig. 4.17 for the maximum proposed superficial velocity (1.1 m/s) and a superficial velocity expected to be near the onset of fluidization (1.5 m/s). The expansion of the fluidized bed (1.5m/s) is indicated by a reduction in total drag force with time. The drag force at the proposed maximum superficial velocity (1.1 m/s) remains at a constant value with time.

FIG. 4.17: COMPARISON OF TOTAL DRAG FORCE PROFILES WITH TIME FOR SUPERFICIAL VELOCITY 1.1 m/s AND 1.5 m/s

4.5. Fluid and Particle Properties

The majority of fluid and particle properties are determined directly from physical conditions in the corresponding experimental setup. Some assumptions in the selected property values are implemented due to lack of information or regard for computational efficiency.

The fluid properties correspond to known properties of air at ambient temperature and pressure. The air is assumed to be incompressible as the pressure fluctuations are expected to be low and a conservative estimate of the maximum fluid velocity yields a Mach number of 0.0065. Table 4.1 contains a comprehensive list of the fluid properties.

TABLE 4.1: FLUID PROPERTIES (AMBIENT AIR)

<u>Property</u>	<u>Value</u>	<u>Units</u>
Fluid Density (ρ_f)	1.2041	kg/m ³
Fluid Viscosity (μ_f)	1.98×10^{-5}	kg/ms

The physical particles are 0.12g airsoft pellets. Airsoft pellets are large, highly spherical, and easy to acquire, making them ideal for comparison between experimental and simulation results. Airsoft particles are made of a blend of synthetic plastics, but lack defined physical property data, possibly due to competition between manufacturers or proprietary blends. Since the precise physical properties are not known, a few assumptions are made, and the effects of these assumptions are investigated. Based on an average value for synthetic plastics, we expect the Poisson ratio to be around 0.45 and, based on previous published DEM simulations, the coefficients of friction and restitution are expected to be around 0.3 and 0.9, respectively.⁷⁵ The particles are modeled with a uniform radius of 3 millimeters and a uniform mass of 0.12g each, as specified by the manufacturer. No rolling friction is prescribed since the particles are known to be highly spherical.⁷⁶ The small variation in density and size

that is expected in any bulk-manufactured pellet blend is ignored in this analysis. The list of particle properties is shown in Table 4.2.

TABLE 4.2: PARTICLE PROPERTIES (AIRSOFT PELLETS)

<u>Property</u>	<u>Value</u>	<u>Units</u>
Particle Radius (R)	0.003	m
Particle Density (ρ_s)	1061	kg/m ³
Poisson Ratio (ν)	0.45	
Coefficient Of Friction (μ)	0.3	
Coefficient Of Restitution(e)	0.9	
Young's Modulus(Y)	1.0×10^7	Pa

Synthetic plastics tend to have a Young's modulus of the order of 10^9 , but this value is reduced to 10^7 to increase computational efficiency. This 100 fold decrease in the Young's modulus value increases the critical time step, and therefore increases the speed of computation, by a factor of 10. The effect of reducing the particle stiffness value is analyzed prior to the grid-refinement study simulations. Two separate methods of analysis are employed to assess this assumption based on published methods.

The first analysis is founded on the claim by Deen *et al.*²² that the simulated Young's Modulus value can be reduced as long as the amount of particle overlap remains reasonable. Deen *et al.*²² states the simulation can handle particle overlaps up to 1% of the particle diameter before the hydrodynamic results are affected. The average overlap of particles in a preliminary simulation is plotted against the superficial velocity in Fig. 4.18. The average overlap remains around 0.2%, but reduces slowly as the particles move farther apart due to the increasing superficial velocity through the bed.

FIG. 4.18: CONTACT-AVERAGED PARTICLE-PARTICLE OVERLAP WITH SUPERFICIAL VELOCITY

The average particle overlap remains far below the published critical value of 1% of the particle diameter, suggesting that the reduced particle stiffness value is acceptable for this application.

In the second analysis, the simulation result with an increased Young's Modulus value of 3×10^8 is compared with the reduced stiffness simulation result. This value of the Young's Modulus is 30 times larger than the proposed reduced value.

The change in drag force due to this larger Young's Modulus value is approximately 0.40%, with the total difference at each superficial velocity value plotted in Fig. 4.19. The actual profiles cannot be visually distinguished, so only the quantitative difference at each superficial velocity is presented. This is a good indication that further increases in the provided Young's Modulus value will not have a large effect on the results.^{21,47}

FIG. 4.19: TOTAL DRAG FORCE CHANGE WITH 30X INCREASE IN YOUNG'S MODULUS VALUE

The assumed coefficient of friction value is similarly analyzed. The simulation results with the assumed value of 0.3 are compared with results from an increased value of 0.4. The increased coefficient of friction results in less than a 0.08% change in drag force, with quantitative differences across the examined values of superficial velocity plotted in Fig. 4.20.

FIG. 4.20: CHANGE IN TOTAL DRAG FORCE WITH INCREASED COEFFICIENT OF FRICTION

The effect of the values of the coefficient of restitution and Poisson ratio for the particles are not investigated. Similar to the coefficient of friction value, they are expected to have negligible effect on the results.

A particle bed with an approximate height of 0.15 meters is comprised of 16,890 total particles. For proper comparison with analytical correlations, the bed must be large enough to exhibit flow through a fixed bed. Ideal fixed beds have axially and radially uniform void fraction and velocity profiles, so pressure drop through the bed is expected to have a linear profile. If the bed is not large enough to properly restrict the flow, inlet effects may result in a non-linear profile. A very large bed that greatly exceeds this minimum height condition will result in high particle numbers and, thereby, reduce the computational efficiency. A bed height of 0.15 meters is proposed as a compromise between these two extremes. The pressure profile along the bed height is shown for two of the lowest velocities in Fig. 4.21, and for the highest examined velocity, in Fig. 4.22. Dashed lines in each of the figures represent a perfectly linear profile between the simulated pressure result at the inlet and atmospheric pressure at the top of the bed.

FIG. 4.21: AXIAL PRESSURE PROFILE THROUGH PARTICLE BED: LOW SUPERFICIAL VELOCITY

FIG. 4.22: AXIAL PRESSURE PROFILE THROUGH PARTICLE BED: HIGH SUPERFICIAL VELOCITY

The axial pressure profiles in Fig. 4.21 and Fig. 4.22 show very little deviation from the expected linear variation. The deviation present in the profiles is not located near the inlet where inlet effects would manifest. Variations in void fraction that naturally occur within the bed are the most likely cause of this deviation from the ideal axial pressure profile. The presence of a linear pressure profile with bed height for all examined velocity values indicates that the bed is large enough to correctly inhibit the fluid flow and produce the desired near-ideal flow through a fixed bed.

4.6. Time-Step Values and Coupling Interval

Time-step values for the CFD and DEM numerical calculation schemes are determined for the most restrictive conditions present in the grid-refinement study for full-range applicability. The CFD and DEM calculations have separate requirements for the critical time step. For accurate time-dependent results, the DEM to CFD time step ratio is desired to be between 50 and 100.¹⁷ The time step values are calculated independently for each solver, and then modified to fit the desired ratio.

The CFD time step calculation is based on the Courant number (Co) which typically is kept below a critical value of 1. For improved accuracy and to ensure numerical stability, we use a more conservative critical value of $Co_{max} = 0.1$. The Courant number expression for flow through a fixed bed is shown in Eq. (4.1):

$$Co = \frac{u \Delta t_{CFD}}{\Delta x} = \frac{u_f \Delta t_{CFD}}{\Delta x} \quad (4.1)$$

The Courant number expression [Eq. (4.1)] requires knowledge of u_f , the interstitial fluid velocity, which can be approximated as the superficial velocity divided by the void fraction. This equation is rearranged to solve for the time step using a conservative estimate of 0.4 for the void fraction as shown in Eq. (4.2):

$$\Delta t_{CFD} = \frac{Co_{max} \Delta x}{u_f} = \frac{0.1 \Delta x}{U/0.4} = \frac{0.04 \Delta x}{U} \quad (4.2)$$

The cell size (Δx) in Eq. (4.2) is the cell length in the direction of the velocity from the finest grid in the grid-refinement study simulation set. Substitution of the smallest grid size and highest superficial velocity into Eq. (4.2) results in a time step value rounded to $\Delta t_{CFD} = 0.0002$ seconds.

The DEM time step is independently calculated using the Rayleigh critical time step [Eq. (3.24)]. The Rayleigh critical time step value is 1.2×10^{-4} seconds. The best-practices suggested DEM time step of 20% of the Rayleigh time step, as shown in Eq. (3.25), is determined to be 2.4×10^{-5} seconds.

The independently developed time step values result in a DEM to CFD time step ratio of approximately 8. This is much lower than generally suggested in the literature, and may not produce accurate results. Hence, the CFD time step is kept at its independently determined value, while the DEM time step is decreased to improve this ratio. The chosen ratio of 50 DEM time steps for each CFD step results in a DEM time step value of 4×10^{-6} , which is 3.33% of the Rayleigh critical time step value. These time step values are conservative, but are expected to lead to relatively computationally efficient simulations. Larger time step values are not investigated since simulation of the full range of desired inlet velocity values requires a very small simulated time of 0.5 seconds.

4.7. Data Output for Post-Processing

Data sets are acquired from the simulation at specified times, and the output interval is a trade-off between computational efficiency and adequate data capturing. Several types of output data are requested at varying intervals to increase computational efficiency while procuring the required data for a wide range of desired analyses. The CFD and DEM data are written separately, with output intervals designed to facilitate reintegration of the data during post-processing.

The CFD solver writes a full set of data every 0.01 seconds and encompasses the entire domain. This complete data set is useful for the analysis of flow variable trends through the bed, such as void fraction and pressure. More frequent output values of the pressure, velocity and void fraction are acquired at specific points along the central axis using the OpenFOAM 'Probe' feature. These limited values are much less computationally expensive to write, and can be analyzed using a simple text interface. The probed values are acquired at every time step (0.0002 seconds) for a thorough check of the pressure-drop convergence with time.

The DEM data set is output every 0.002 seconds, 5 times more often than the full CFD data set. The DEM data set is used to check for drag-force convergence with time; this is essential for correct, repeatable results. The DEM data set is also used to check for excessive particle overlap, and the results suggest that the assumption of reduced particle stiffness is not detrimental to simulation accuracy. The DEM data can be analyzed quantitatively using a text interface, or qualitatively using a visualization tool.

Both sets of data are analyzed using a text interface as well as the open-source post-processing tool Paraview. Paraview is standard in the CFDEM installation, and is a useful open-source tool for visualization and data analysis.

Chapter 5

Results and Discussion

Chapter 5 describes and discusses the simulation results and grid-refinement study results. The input parameters for the simulations have been checked and results reported in Chapter 4. The simulation results in this chapter are checked individually to ensure steady state attainment of pressure drop and total drag force before the results are included in this study.

Section 5.1 through Section 5.3 present simulation results with the Gidaspow drag correlation since it is expected to give the best comparison with the Ergun equation results. The solution trend of resultant total drag force with grid size and drag force with velocity for each grid is examined in Section 5.1. An observation of different drag profile shapes with superficial velocity for the different grid results led to the curvature investigation in Section 5.1.1.

Grid-refinement studies are performed for 60 combinations of the 13 grid solutions, and the results are reported in Section 5.2. An example of a single group grid-refinement study is given in the introduction to Section 5.2, followed by an explanation of the procedure for determining which grid combinations are examined in Section 5.2.1. The frequency of convergence and convergence types are described in Section 5.2.2. The offset method for quantitative comparison of expected numerical error and extrapolated solution error from the grid-refinement study is described in Section 5.2.3.

An optimal grid size for this modeling application is investigated in Section 5.3. The methods of analysis include investigation of the solution trend in Section 5.3.1, trends of regression coefficients in Section 5.3.2, and offset method results in Section 5.3.3. An independent method of analysis which does not require the use of an analytical correlation is proposed and applied in Section 5.3.4. The

results in Sections 5.3.1 through 5.3.3 are tallied in Section 5.3.5. The resulting optimal grid size of 1.94 particle diameters is shown to match with the independently determined optimal size in Section 5.3.4.

The Gidaspow drag correlation simulation results are compared to Koch-Hill and Di-Felice drag correlation simulation results in Section 5.4. Comparison is performed using methods similar to the optimal cell size analysis, including solution trend in Section 5.4.1, regression coefficient analysis in Section 5.4.2, offset method results in Section 5.4.3, and the independent method of average GCI value in Section 5.4.5. The convergence frequency of grid-refinement studies for simulations from each of the drag correlations is compared in Section 5.4.4. Results of the correlation comparisons are discussed in Section 5.4.6.

5.1. Solution Trend

The solution trend is analyzed several different ways to investigate different characteristics of the solution trend with changing grid size. The first method of analysis involves examination of the drag-force results across the range of non-dimensionalized grid size. Qualitative error and solution behavior with grid size are investigated by plotting the drag-force results at a chosen velocity with the grid size and comparison of the results with the Ergun equation drag force. Fig. 5.1 shows the solution trend across all of the analyzed grids at a relatively high velocity of 1 m/s, while Fig. 5.2 is the same for a lower velocity of 0.5 m/s.

FIG. 5.1: SOLUTION TREND AT VELOCITY OF 1 M/S

FIG. 5.2: SOLUTION TREND AT VELOCITY OF 0.5 M/S

A comparison of Fig. 5.1 and Fig. 5.2 shows similar solution trends with some unique features. The solution trend does not appear to converge as the ratio of grid size to particle diameter is reduced towards the lowest acceptable ratio of unity. The trend also diverges as the cell size becomes much larger than the cell size. The solution does appear to converge towards the Ergun equation result for a cell size between 2 and 3 particle diameters.

A more comprehensive representation of the accuracy of each simulation is the resulting total error. In order to treat errors throughout the profile in the same manner, the total difference between the simulation results and Ergun equation result is calculated and divided by a sum of the expected Ergun equation results. In this manner, relatively small errors in the low range of the profile are not magnified due to the relatively small expected drag in this range. The total error is plotted against the non-dimensionalized grid size in Fig. 5.3.

FIG. 5.3: TREND OF TOTAL SOLUTION ERROR WITH GRID SIZE

Convergence towards the solution appears to occur in Fig. 5.3 near a grid size of 2 particle diameters. The simulation with the least error has a grid size to particle diameter ratio of 1.94, and is within 1.4% of the expected Ergun equation profile.

The presence of oscillations throughout the solution trend was not expected and the cause of these ‘spikes’ is unknown. Possible causes of this large variation include changes in porosity field calculated average, porosity field standard deviation and skewness in each computational mesh. No definite correlation between any of these causes and the error variation are established in this work. The porosity field variation with grid size is included in Appendix A where large variations appear similar to variations in the solution trend total error. The ratio of maximum grid length to minimum grid length is plotted for each grid in Appendix A. Large maximum to minimum grid length values appear to correlate with large error values. An additional simulation was run for a grid size to particle diameter ratio of around 1.89. The solution for the grid-refinement study at this level of refinement is calculated on a relatively highly skewed grid (maximum to minimum grid length value of 2.05). The additional solution calculated at a similar level of refinement on a less skewed grid (maximum to minimum grid

length of 1.55) included an almost four-fold reduction in error (reduced total error from 3.74% to 1.04%).

The simulation results from each of the grids are also analyzed separately. A separate analysis reveals areas of over- and under-prediction in the drag force profile with changing superficial velocity. In Fig. 5.4, the drag profile results from the least error solution ($R = 1.94$) are compared with the Ergun equation profile.

FIG. 5.4: COMPARISON OF DRAG PROFILE FOR SIMULATION AT $R = 1.94$ AND ERGUN EQUATION RESULTS

The solution results are very similar to the Ergun equation profile, but with some under-prediction of the drag force at the higher superficial velocity values. This analysis method can be used to compare multiple simulation results with the expected Ergun equation profile. The highest error result at $R = 3.80$ is included in Fig. 5.5 for comparison with the Ergun equation profile.

FIG. 5.5: COMPARISON OF DRAG PROFILE FOR SIMULATION AT R=1.94, R=3.80 AND ERGUN EQUATION

The two simulation solutions in Fig. 5.5 are largely different in value and predicted relationships of drag force with superficial velocity. Comparison of simulation results to the Ergun equation and to each other reveals different levels of profile curvature with regards to velocity. This is discussed further in the next subsection.

5.1.1. Curvature

The observed difference in curvature with velocity in the simulation drag profiles is critical for analysis since the Ergun equation specifically states the expected relationship of the drag force to the superficial velocity. A regression analysis is performed on the simulation results to obtain coefficients of velocity and velocity squared, to be compared with the Ergun equation coefficient results. The desired regression coefficients are based on the reduced version of the Ergun equation shown in Eq. (5.1).

$$F_{D,total} = C_1 U + C_2 U^2 \quad (5.1)$$

Values of the regression coefficients calculated from simulation results are compared with the Ergun equation results from Eq. (2.9) in Fig. 5.7 and Fig. 5.8. The regression is performed in Microsoft Excel for each simulation result and a sample of the Excel output is shown in

Fig. 5.6.

SUMMARY OUTPUT								
Regression Statistics								
Multiple R	0.999997							
R-Square	0.999993							
Adjusted R-Square	0.888882							
Standard Error	0.015511							
Observations	11							
ANOVA								
	df	SS	MS	F	Signif. F			
Regression	2	333.1037	166.5519	692227.6	1.11E-21			
Residual	9	0.002165	0.000241					
Total	11	333.1059						
	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	0	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A
X Variable 1	1.490448	0.027715	53.77725	1.34E-12	1.427752	1.5531	1.4277	1.5531
X Variable 2	7.494839	0.031182	240.3575	1.9E-18	7.424301	7.5653	7.4243	7.5653

FIG. 5.6: SAMPLE REGRESSION RESULTS FROM MICROSOFT EXCEL

The regression results for each drag force profile exhibit large R-square values and low error, indicating the simulation profiles are accurately modeled by the regression function. The simulation-based coefficients are plotted against the expected Ergun equation coefficient for the velocity in Fig. 5.7 and for the velocity squared in Fig. 5.8.

FIG. 5.7: COEFFICIENT OF VELOCITY TREND WITH GRID SIZE RATIO

FIG. 5.8: COEFFICIENT OF VELOCITY SQUARED TREND WITH GRID SIZE RATIO

The trends in Fig. 5.7 and Fig. 5.8 do not converge towards the Ergun equation values at the same grid ratio as the solution trend does in Fig. 5.3. Therefore, simple convergence towards to the solution may not indicate accurate representation of the relationship between velocity and total drag. This is one of the many reasons that a grid-refinement study is required to determine the convergence

of a solution trend. Low total error in a single simulation does not guarantee accurate representation of the physics involved in the problem. Convergence towards the correct solution with decreasing cell size in a certain range is the best indication that the simulation is correctly designed for the problem, and solved with stable, well-applied numerical schemes.

5.2. Grid-Refinement Study

A grid-refinement study consisting of three chosen grids is completed using the drag force at each value of superficial velocity individually. This allows recognition of different trends of convergence for the drag force results at each velocity value of interest. The results are grouped in two categories – low velocity results (0.1 – 0.5 m/s) and high velocity results (0.6 – 1.1 m/s), as determined from similar solution trends seen in the data at these velocity ranges.

The apparent rate of convergence of the solution trend at each velocity value is calculated individually, and the minimum and maximum rate over all of the velocities is reported. The R_k value is calculated as part of the grid-refinement study and the minimum and maximum R_k values are also reported to determine the convergence regimes present in the solution trend. The Grid Convergence Index (GCI) is reported as an average over the calculated values at each velocity value.

The extrapolated solution for total drag force at each velocity value is compared to the Ergun equation value. The absolute error is calculated at each velocity value and then averaged over the velocity range. This is reported as the average absolute extrapolated solution error.

A sample grid-refinement study result is shown in Table 5.1. The grid-refinement study results are determined by iteration with the apparent rate of convergence as the iterated value. These results are combined by averaging the values over the different velocity ranges to form the grouped results shown in Table 5.2, and will be used for the remainder of the analysis.

TABLE 5.1: COMPLETE RESULTS FROM SINGLE GROUP GRID-REFINEMENT STUDY

<u>Velocity</u> (m/s)	<u>Drag Force Values from</u> <u>Grid Solutions</u>			<u>Convergence</u> <u>Category Criteria</u>		<u>Grid-Refinement Results</u>		Extrapolated Solution Error
	ϕ_1	ϕ_2	ϕ_3	R_k	p	GCI	Extrapolated Solution	
0.1	0.23	0.24	0.24	-0.11	4.49	2.40%	0.22	2.45%
0.2	0.62	0.67	0.66	-0.12	4.32	2.52%	0.61	4.59%
0.3	1.19	1.28	1.27	-0.13	4.16	2.70%	1.16	6.22%
0.4	1.92	2.06	2.04	-0.13	4.10	2.74%	1.88	7.21%
0.5	2.82	3.02	2.99	-0.14	3.99	2.86%	2.75	7.44%
0.6	3.88	4.16	4.12	-0.15	3.78	3.11%	3.79	6.51%
0.7	5.11	5.47	5.41	-0.17	3.62	3.35%	4.97	3.83%
0.8	6.53	6.96	6.88	-0.19	3.36	3.49%	6.35	3.56%
0.9	8.10	8.62	8.51	-0.21	3.17	3.78%	7.86	0.78%
1	9.96	10.46	10.31	-0.29	2.59	4.11%	9.63	4.45%
1.1	11.76	12.46	12.27	-0.27	2.71	4.56%	11.33	14.36%

TABLE 5.2: AVERAGED RESULTS FROM SINGLE GROUP GRID-REFINEMENT STUDY

<u>Grid Size Ratios</u>	
r_{21}	1.43
r_{32}	1.19
<u>Low Velocity Range Averages</u>	
Error	7.41%
GCI	2.65%
<u>High Velocity Range Averages</u>	
Error	0.98%
GCI	3.77%
<u>Convergence Category Definitions</u>	
$P_{(min)}$	2.59
$P_{(max)}$	4.49
Minimum R_k	-0.29
Maximum R_k	-0.11

The results for the group grid-refinement study in Table 5.2 are analyzed by categorization of convergence type. The minimum and maximum R_k values in Table 5.2 are negative but have a magnitude less than unity. This range of R_k indicates the oscillatory convergence for the drag force

trends in each velocity range. While oscillatory convergence is not the ideal convergence category, the apparent order of accuracy (p) range indicates the convergence is relatively fast. Since rapid convergence is expected from the solution trends, the GCI values for both velocity ranges are low. In the low velocity range, the extrapolated solution error relative to the Ergun equation is larger than the calculated GCI value, indicating the presence of modeling error. In the high velocity range, the GCI value is larger than this error, which suggests the error in the solution can be accounted for by the numerical error. Each group grid-refinement study is examined in this manner, and grouped by the convergence trend and observed order of accuracy.

5.2.1. Grid Combinations

With 13 grids, there are 286 possible combinations for grid-refinement studies with only one main limitation. Standard practice for CFD grid-refinement studies is to limit the ratio between grid sizes to be at least 1.3. We expect a very limited range of cell size in which convergence occurs, not the relatively large asymptotic range present in most CFD simulations. Hence, the minimum grid size ratio is reduced to 1.15.

During the completion of grid-refinement studies, it was also found that the refinement ratio between the first two grids must be similar to the refinement ratio between the subsequent two grids. Large differences in these ratios resulted in calculated apparent orders of accuracy that were too large (converging towards infinity) or too small (nearly zero). The apparent order of accuracy was checked for each grid-refinement study and any study nearing these conditions was not included in the final analysis.

As a result of these stipulations, a total of 60 grouped grid-refinement studies were performed. Each group of grid-refinement studies consisted of studies at 11 chosen velocity values as shown in Table 5.1. The results were consolidated into one result per velocity group as shown in Table 5.2.

5.2.2. Frequency of Convergence

A converging trend is defined as a GCI less than 10%, which indicates that the finest grid solution is expected to have less than 10% numerical error. As shown in Fig. 5.9, of the 60 total studies performed, 17 (28%) showed convergence in the high velocity category, 16 (27%) showed convergence in the low velocity category. These convergence regimes overlap with 15 (25%) total simulations showing convergence in both categories. Therefore, in future applications, we expect that more than 3 grid solutions will be required to find a converging solution trend. Grid-refinement studies for granular-fluid flow simulations are expected to require significant computational resources.

FIG. 5.9: FREQUENCY OF CONVERGENCE FOR GIDASPOW GRID-REFINEMENT STUDIES

The convergence trends can be analyzed with better respect to the solution trends using the calculated R_k value. The corresponding convergence or divergence regime for each range of R_k is described in Section 0, with an overview in Fig. 2.4. The frequency of the worst convergence type seen in each group grid-refinement study is shown in Fig. 5.10.

FIG. 5.10: FREQUENCY OF CONVERGENCE TYPE IN GRID-REFINEMENT STUDIES

Oscillatory divergence is observed in 47% of the grid-refinement studies. The ideal monotonic convergence is present in only 15% of the grid-refinement studies. A diverging trend is seen in at least one region (high velocity or low velocity) for 77% of the grid-refinement studies. The average extrapolated solution error and GCI values are calculated for each convergence type and compared in Fig. 5.11.

FIG. 5.11: AVERAGE EXTRAPOLATED ERROR AND GCI FOR EACH CONVERGENCE TYPE

Oscillatory divergence results in the highest values of GCI and extrapolated solution error, followed by monotonic divergence. Monotonic and oscillatory convergence result in significantly lower GCI and extrapolated solution error values.

5.2.3. Offset Method

Another method of analysis for the grid-refinement studies is comparison of a quantity termed 'offset.' Offset is defined as the difference between the actual error of the extrapolated solution and the expected numerical error, or GCI. Reasons for the presence and magnitude of offset can include additional numerical errors that were not recognized by the grid-refinement study (*e.g.* numerical error from discretization of time) and modeling errors with respect to the predicted Ergun equation results. Fig. 5.12 shows the actual numerical error in the extrapolated solution plotted against the GCI to give a graphical representation of offset.

FIG. 5.12: EXTRAPOLATED SOLUTION ERROR VS. GCI FOR SIMULATIONS WITH GIDASPOW DRAG CORRELATION

Qualitatively the offset amount for this set of simulations can be described as minimal, since most extrapolated solution errors shown in Fig. 5.12 are close to or below the expected numerical error (GCI). A quantitative representation of offset is taken as the average offset over all grid-refinement

study results with GCI values less than 50%. As seen in Fig. 5.12, some studies contain extrapolated error values of lesser magnitude than the GCI value, and these are included in the total offset average as a zero value offset. The average offset in the low velocity range is 2.66%, for high velocity range is 2.56%, and overall is 2.61%. These low offset values indicate very few modeling errors since the solution trend is converging towards the known analytical solution. This result is expected since the Gidaspow drag correlation is an exact representation of the Ergun equation for the effective void fraction range. Low offset is a good indication that the grid-refinement study is able to accurately capture the solution trends and is, therefore, useful for this application.

5.3. Optimal Cell Size

An additional goal of this study is to develop methods to determine the optimal cell size for accurately capturing the physics in a granular-fluid flow. This method should be applicable to all granular fluid flows, and ideally should consider a non-dimensionalized quantity that can be employed across similar applications. The need for a defined optimal cell size as well as a description of previous attempts to define this quantity was discussed in Section 3.3.3. To approximate the optimal cell size for this application, three different approaches are used, and their results are compared. These approaches are: an analysis of the solution trend, analysis of the regression coefficients from each solution and application of the grid-refinement study results.

5.3.1. Solution Trend

Analysis of the solution trend is simple, and can be accomplished by a plot of total solution error with cell size. This plot is included in Section 5.1 as Fig. 5.3. The three grid sizes resulting in the least amount of error can be easily determined, and are ranked by error in Table 5.3.

TABLE 5.3: GRID SIZE RATIOS RESULTING IN LEAST ERROR WITH ERGUN EQUATION DRAG FORCE VALUES

<u>Ratio of Grid Size to Particle Diameter</u>	<u>Total Solution Error</u>
1.94	1.38%
2.14	2.13%
1.74	2.43%

5.3.2. Regression Coefficients

A similar method of results comparison requires the use of a regression function as described in Section 5.1.1. The analytical solution and the simulation results are represented in terms of coefficients of velocity and velocity squared. These coefficient results are compared in Fig. 5.7 and Fig. 5.8 of

Section 5.1.1. The three simulation results closest to the coefficient values are shown in Table 5.4 for the coefficient of velocity, and in Table 5.5 for the coefficient of velocity squared.

TABLE 5.4: GRID SIZE RATIOS RESULTING IN LEAST ERROR WITH ERGUN COEFFICIENT OF VELOCITY

<u>Ratio of Grid Size to Particle Diameter</u>	<u>Calculated Coefficient Error</u>
1.46	4.18%
1.60	4.46%
1.28	11.15%

TABLE 5.5: GRID SIZE RATIOS RESULTING IN LEAST ERROR WITH ERGUN COEFFICIENT OF VELOCITY SQUARED

<u>Ratio of Grid Size to Particle Diameter</u>	<u>Calculated Coefficient Error</u>
1.89	0.41%
2.38	0.66%
2.79	1.15%

It is interesting to note that the grid size ratios resulting in the best agreement with the Ergun equation drag values at each velocity do not necessarily have the best agreement with the Ergun equation coefficients of velocity and velocity squared. This illustrates why multiple methods of analysis are needed to determine the optimal grid size for accurate results.

5.3.3. Offset Method

A grid-refinement study is used in typical CFD applications to determine the cell size at which the solution is mesh independent. CFDEM does not exhibit the traditional monotonic convergence (asymptotic region) seen in CFD applications, and is expected to have critical grid sizes as R becomes too large and as R becomes too small. While this complicates the application and analysis of grid-refinement studies, the results can still be used to suggest an optimal grid size.

The grid-refinement results are used in unique ways to analyze this complicated scenario. Fig. 5.13 is a plot of the average offset defined in Section 5.2.3 against the grid size to particle-diameter ratio of the finest grid in the grid-refinement study.

FIG. 5.13: TREND OF AVERAGE OFFSET WITH FINEST GRID NON-DIMENSIONALIZED CELL SIZE

This trend is very similar to what is expected, with the exception of the peak at $R = 1.89$. The reason for this peak was investigated, but no definitive reason was identified. The reduction in number of grid-refinement studies that could be performed as the grid size was increased is the only likely cause. The finest grid solution in this study ($R = 1.28$) is the finest grid in 20 grid-refinement studies, while the grid solution in question ($R = 1.89$) is the finest grid in only five studies.

Though the variation in number of grid-refinement studies performed for each grid may cause some error in the trend, three grids with the lowest offset are noted in Table 5.6.

TABLE 5.6: GRID SOLUTIONS WITH LEAST AVERAGE OFFSET

<u>Ratio of Grid Size to Particle Diameter</u>	<u>Average Offset</u>
1.94	0.58%
1.74	0.66%
1.60	1.37%

5.3.4. Alternate Methods of Optimal Cell Size Determination

Since an analytical solution is known for the present case, these analyses provide a way to determine which grid leads to the most accurate solution. In most models, an analytical expression for the drag force is not available, and other analysis methods are needed to determine optimal cell size. For this reason, we apply the results of the grid-refinement study to determine if this is a useful tool for choosing the optimal cell size when no analytical solution is available. The convergence frequency for each grid used as the finest grid for at least one grid-refinement study is plotted against the non-dimensionalized cell size in Fig. 5.14. It is important to note that the number of grid-refinement studies corresponding to each grid increases as the grid cell size decreases. The coarsest grid result included in Fig. 5.14 serves as the finest grid in only one grid-refinement study. This singular result is included here for reference, but this grid will not be included in the future analysis.

FIG. 5.14: TREND OF CONVERGENCE FREQUENCY WITH NON-DIMENSIONALIZED CELL SIZE OF FINE GRID

From the trend in Fig. 5.14, we recommend in this case that grid-refinement studies should only be performed when the fine grid has a cell size to particle diameter ratio greater than 1.60. The three

examined grids below this threshold resulted in less than 20% convergence frequency when used as the finest grid in a grid-refinement study.

The convergence frequency is plotted against the average offset in Fig. 5.15 to assess whether a relationship exists between convergence frequency and the presence of modeling errors with respect to the Ergun equation correlation.

FIG. 5.15: AVERAGE OFFSET VALUES WITH CONVERGENCE FREQUENCY

No clear trend exists in Fig. 5.15 between the average offset and convergence frequency. For this case, the convergence frequency cannot be used to predict relative solution accuracy.

From Fig. 5.14, it is clear that each grid used as the finest grid in multiple grid-refinement studies experiences less than 100% convergence. Grid-refinement studies performed over diverging solution trends produce error predictions (GCI) of up to 5000%! The GCI values are the expected numerical error in the finest grid solution, so the GCI from well-behaved solution trends is useful for predicting the expected numerical error. The actual error in the finest grid solution compared to the Ergun equation result is plotted against the average GCI values in Fig. 5.16. The only GCI values used for averaging are less than 50% as this is taken as the metric for a well-behaved solution trend. While a GCI value of 50%

is very large, this criterion is proposed as a maximum acceptable value and most of the GCI values for the included grid refinement studies are significantly smaller than this critical value.

FIG. 5.16: EXPECTED NUMERICAL ERROR COMPARED WITH FINEST GRID ERROR

A positive correlation between average GCI and finest grid error is calculated with 95% confidence. This correlation explains more than 80% of the total variation in the finest grid error. The average GCI of well-behaved solutions is proposed as a prediction mechanism for finest grid error.

This method of error prediction is recommended when analytical solutions or experimental data are not available for error calculation. From this procedure with no analytical solution data, the recommended cell size is 1.94 particle diameters with the lowest average GCI of 3.28%.

5.3.5. Choice of Cell Size

The results presented in Sections 5.3.1 to 5.3.3 are tabulated, and the resulting recommendations are quantitatively presented by assigning values to each recommendation. In each method, the grid size ratio with the least error is awarded one point. The grid size corresponding to the second closest result is awarded half a point while the grid corresponding to the third best result is only

awarded one quarter of a point. This is an arbitrary point system with no physical basis, and is used only to tally the recommendations. The results shown in Fig. 5.17 reveal that a cell size to diameter ratio of 1.94 is the most recommended result, and cell sizes between 1.46 and 1.89 are also highly recommended. Cell sizes above 1.94 particle diameters per cell size are not as highly recommended due to higher resulting error.

FIG. 5.17: FREQUENCY OF RECOMMENDATION FOR CELL SIZE BASED ON CHOSEN POINT SYSTEM

For this application and numerical solution procedure, we recommend a cell size of 1.94 particle diameters. This is a first attempt at determining a general method to calculate optimal grid size for granular flow simulations conducted in the present work. The resulting ratio of 1.94 particle diameters per cell length is not expected to be applicable to general granular flow simulations. This proposed method is suggested for use in general simulation to develop a more rigorous non-dimensional optimal grid size definition. While we treat the optimal cell size in this study as a multiple of the particle diameter, it may also be a function of other bed or flow properties such as column diameter, velocity or particle residence time.

5.4. Comparison of Drag Correlations

Simulations across the same 13 grids used in the earlier analyses are repeated with the Koch-Hill and Di-Felice drag correlations. The results of each drag correlation are compared using the solution trend and curvature analysis. Grid-refinement studies are performed for the same grid combinations as the first grid-refinement study, and comparisons are made based on average offset, convergence frequency and average GCI values. Conclusions about the applicability of each of these drag correlations to simulate fixed-bed flow are drawn from these analyses, and compared with the predicted applicability.

5.4.1. Solution Trend

The solution trend of the Koch-Hill drag correlation simulation results is shown in Fig. 5.18. The Koch-Hill correlation analytical under-prediction of the Ergun equation is immediately evident in the high resultant error. The lowest error grid solution has 3.1% total error at a grid size of 3.8 particle diameters.

FIG. 5.18: TREND OF TOTAL SOLUTION ERROR WITH CELL SIZE FOR KOCH-HILL SIMULATION RESULTS

The total drag force profile with superficial velocity is shown in Fig. 5.19 for the best performing and worst performing Koch-Hill simulation with a cell size to particle diameter ratio of 3.8 and 1.28, respectively.

FIG. 5.19: COMPARISON OF TOTAL DRAG FORCE WITH SUPERFICIAL VELOCITY FOR KOCH-HILL SIMULATION RESULTS

The worst performing simulation drag profile ($R = 1.28$) features the expected under-prediction, especially at relatively high superficial velocities. The best-performing simulation drag profile ($R = 3.80$) over-predicts the Ergun result at mid-range superficial velocities, and under-predicts the drag force at higher superficial velocities.

The solution trend for the Di-Felice correlation implementation is shown in Fig. 5.20. The simulation results are very close to the Ergun equation result for a grid size near two particle diameters.

FIG. 5.20: TREND OF TOTAL SOLUTION ERROR WITH CELL SIZE FOR DI-FELICE SIMULATION RESULTS

The grid solution with the least error and the grid solution with the greatest error are compared to the Ergun equation result in Fig. 5.21. The grid solution at $R = 2.14$ has the least error with only 1.94% error when compared to the Ergun equation result. The greatest error grid solution is located at $R = 3.80$ with a total error of 28.2% of the Ergun equation values.

FIG. 5.21: COMPARISON OF DRAG FORCE PROFILE WITH SUPERFICIAL VELOCITY FOR DI-FELICE SIMULATION RESULTS

The solution with the greatest error in Fig. 5.21 over-predicts the drag force profile with superficial velocity. This is unexpected since the analytical application of the Di-Felice correlation resulted in a large under-prediction of the Ergun equation values. This discrepancy indicates that the porosity field calculated on this grid likely differs greatly from the expected values.

5.4.2. Regression Coefficients

The regression coefficients from Koch-Hill and DiFelice correlation simulations are compared to the known Ergun coefficients in the same manner as in Section 5.1.1. The Koch-Hill simulation regression coefficients with cell size are shown in Fig. 5.22 and Fig. 5.23 for coefficient of velocity and coefficient of velocity squared, respectively.

FIG. 5.22: KOCH- HILL COEFFICIENT OF VELOCITY TREND WITH GRID SIZE RATIO

FIG. 5.23: KOCH-HILL COEFFICIENT OF VELOCITY SQUARED TREND WITH GRID SIZE RATIO

The resulting coefficient of velocity values greatly over-predict the Ergun coefficient as shown in Fig. 5.22, while the resulting coefficient of velocity squared values under-predict the Ergun value as shown in Fig. 5.23. The Koch-Hill correlation clearly does not capture all of the physics in the flow through a fixed bed. This is expected since the Koch-Hill correlation was developed for fluidized bed conditions and is not designed to represent flow through fixed beds.

The Di-Felice regression coefficients are compared for coefficient of velocity and coefficient of velocity squared in Fig. 5.24 and Fig. 5.25, respectively.

FIG. 5.24: DI-FELICE COEFFICIENT OF VELOCITY WITH GRID SIZE RATIO

FIG. 5.25: DI-FELICE COEFFICIENT OF VELOCITY SQUARED WITH GRID SIZE RATIO

The calculated coefficients from Di-Felice simulation results are very close to the Ergun equation result in certain ranges. The coefficient of velocity in Fig. 5.24 approaches the Ergun equation value at a much lower value than the range of least total solution error. Alternately, the coefficient of velocity squared in Fig. 5.25 remains near the Ergun equation coefficient value in the same range as low total solution error is encountered.

5.4.3. Offset Method

The results are analyzed using the grid-refinement study results by the offset method in the manner of Section 5.2.3. The extrapolated solution error is compared to the calculated GCI for the Koch-Hill simulations in Fig. 5.26.

FIG. 5.26: EXTRAPOLATED SOLUTION ERROR VS. GCI FOR SIMULATIONS WITH KOCH-HILL DRAG CORRELATION

Fig. 5.26 can be compared with Fig. 5.12 in Section 5.2.3 for the Gidaspow drag correlation model results. The Koch-Hill results have a much greater amount of offset than the Gidaspow results; this indicates significantly larger modeling errors in the Koch-Hill correlation application.

Grid-refinement studies for the Di-Felice simulations exhibit a much smaller average offset value. The comparison of extrapolated solution error with GCI in Fig. 5.27 is similar to that of the Gidaspow model application in Fig. 5.12 of Section 5.2.3.

FIG. 5.27: COMPARISON OF EXTRAPOLATED SOLUTION ERROR AND GCI FOR DI-FELICE SIMULATIONS

Since the offset amount for the Di-Felice and Gidaspow model applications is similar, the extrapolated solution correlation with the GCI is plotted for all of the investigated drag correlations in Fig. 5.28.

FIG. 5.28: COMPARISON OF EXTRAPOLATED SOLUTION ERROR WITH GCI FOR EACH DRAG CORRELATION IMPLEMENTATION

The average offset in grid-refinement studies with less than 50% expected numerical error for each drag correlation is quantitatively compared in Table 5.7.

TABLE 5.7: AVERAGE OFFSET FOR EACH DRAG CORRELATION IMPLEMENTATION

<u>Drag Correlation</u>	<u>Average Offset (%)</u>
Gidaspow	2.61
Koch-Hill	9.73
Di-Felice	3.12

The Gidaspow drag correlation results in the least amount of offset, followed closely by the Di-Felice drag correlation implementation. The Koch-Hill drag correlation simulation results contain a much larger average offset, and are therefore expected to exhibit much greater modeling errors.

5.4.4. Convergence Frequency

The frequency of convergence and type of convergence are compared in the grid-refinement studies for each of the drag correlation applications. The Gidaspow convergence frequency is given in Fig. 5.9 and Fig. 5.10. The Koch-Hill correlation application results in the grid-refinement convergence frequency shown in Fig. 5.29, and the convergence type frequency shown in Fig. 5.30.

FIG. 5.29: FREQUENCY OF CONVERGENCE FOR KOCH-HILL GRID-REFINEMENT STUDIES

FIG. 5.30: FREQUENCY OF CONVERGENCE TYPES FOR KOCH-HILL GRID-REFINEMENT STUDIES

Grid-refinement studies for the Koch-Hill simulation results exhibit higher frequency of convergence and higher amount of ideal (monotonic) convergence trends.

The Di-Felice correlation application results in significantly less convergence as seen in Fig. 5.31. Over 75% of the solution trends examined are seen to diverge.

FIG. 5.31: FREQUENCY OF CONVERGENCE FOR DI-FELICE GRID REFINEMENT STUDIES

The majority of solution trends exhibit monotonic divergence, and only 25% of the solution trends exhibit the ideal monotonic convergence as seen in Fig. 5.32.

FIG. 5.32: FREQUENCY OF CONVERGENCE TYPES FOR DI-FELICE GRID-REFINEMENT STUDIES

5.4.5. Average GCI Value

Finally, the average GCI value is compared with the total solution error from the finest grid in the grid-refinement study. As explained in Section 5.3.4, this is an attempt to use the average GCI value from grid-refinement studies with well-behaved solution trends to predict the relative error in the finest grid.

The error in the finest grid compared to average GCI value is shown in Fig. 5.33. The ‘well-behaved’ solution trends in this case are based on a critical maximum GCI of 50%.

FIG. 5.33: EXPECTED NUMERICAL ERROR AS A PREDICTOR OF FINEST GRID ERROR: KOCH-HILL CORRELATION

The trend in Fig. 5.33 is not as obvious as the relationship between finest grid error and average GCI for the Gidaspow drag correlation application in Fig. 5.16 of Section 5.3.4. The trend in Fig. 5.33 does show a positive correlation between the average GCI and finest grid error, but this correlation explains less than 50% of the variation in the solution error of the finest grid. The expected intercept of the correlation is around 10%, indicating that near-zero values of GCI are expected to correspond to 10% solution error. This is another clear indication of modeling errors, with respect to the Ergun equation correlation, in the Koch-Hill drag correlation application to flow through fixed beds.

The error in the finest grid is compared to the average GCI value in Fig. 5.34 from the grid-refinement studies for the Di-Felice drag correlation.

FIG. 5.34: EXPECTED NUMERICAL ERROR AS A PREDICTOR OF FINEST GRID ERROR: DI-FELICE CORRELATION

The average GCI appears to be a good predictor of the finest grid solution error for this drag correlation application, with a simple linear correlation accounting for nearly 85% of the variation.

5.4.6. Overall Comparison

The Gidaspow and Di-Felice correlations show the best comparison with the known Ergun equation solution. The Koch-Hill correlation exhibits large error, and largely under-predicts the solution. The solution trend and regression method provide qualitative comparisons to first identify these trends. The offset method is found to be a good quantitative comparison tool, with the Gidaspow correlation resulting in the least amount of offset. The convergence frequency varies greatly between the three correlation applications, and does not appear to be related to the applicability of the drag correlation. The overall GCI value is found to be a very good predictor of finest grid error in grid-refinement studies for the applicable drag correlations (Gidaspow, Di-Felice). The GCI is only a decent predictor of finest

grid error for the Koch-Hill drag correlation. Finally, a correlation is attempted in Fig. 5.35 between all of the finest grid error and average GCI values across the drag correlations.

FIG. 5.35: AVERAGE GCI AS A PREDICTOR OF FINEST GRID ERROR ACROSS MULTIPLE DRAG CORRELATION

IMPLEMENTATIONS

Less than 20% of the finest grid error is explained by the correlation with average GCI. Therefore, while the average GCI value is a helpful tool for determining optimal grid size, it is not able to distinguish relative errors between the correlation application results. The offset method, which requires an analytical solution or experimental data, is the recommended method for drag correlations selection.

Chapter 6

Conclusion

Simulations over a range of grid sizes were performed using an open-source computational fluid dynamics – discrete element method (CFD-DEM) coupling to model air flow through a fixed bed of large spherical particles. The simulation procedure was repeated for two empirical drag correlations designed for the regime of flow through a fixed bed and for a separate drag correlation developed from Lattice-Boltzmann Simulations to model the fluidized-bed regime.

The full solution trend with grid size was much more complicated than expected, with large variations throughout the profile. Large variations in the solution were seen at relatively large and relatively small grid sizes as was expected from the published literature. The existence of two critical grid sizes bounding the somewhat-asymptotic range is an added complexity that must be accounted for in future research. The comparison of only two grid solutions is not sufficient since each grid could conceivably violate one of the critical size values.

This study constitutes the first application of a grid-refinement study to an unresolved CFD-DEM simulation. A comparison of expected numerical error and extrapolated solution error from the grid-refinement study, termed the offset method, was found to be a useful quantitative comparison for modeling design parameters such as optimal cell size determination and comparison of drag correlations. The frequency of convergence was found to be low, even for appropriately designed simulations. The frequency of convergence and frequency of convergence types were found to have no relation to the model applicability.

The average expected numerical error (GCI) values in the present study were very large. Future studies with less variation in cell shape and more levels of refinement are needed to determine ways to reduce this uncertainty in the results. From the present study, the average GCI value from relatively

well-behaved solutions ($GCI < 50\%$) was found to be a good predictor of the finest grid solution error. This correlation is very useful since it does not require an analytical solution or experimental data. The average GCI was found to be a useful tool in determining the optimal cell size.

A method for determination of optimal cell size was demonstrated using the solution trend analysis, regression coefficients, and the offset method. A similar method was demonstrated for the choice of drag correlations using the solution trend, regression coefficients and the offset method. The grid-refinement study results were shown to be useful for quantitative comparison in both of these methods.

From these results, we strongly recommend further research into the solution trend of granular flow simulations with cell size. The confirmation in this work of the existence of two critical cell sizes and the large amount of variation present in the solution trend are cause for concern in the validation of granular-fluid interaction simulations. Grid-refinement study results, while computationally expensive, were shown to be useful for informed modeling decisions, comparison of relative errors and uniform error reporting.

6.1. Future Work

While the results of the present study are very encouraging for the development of uniform reporting criterion for granular-fluid interaction simulations, the grid-refinement study is only applied to one unique system. This technique must be applied more broadly to determine its effectiveness and to develop more general methods of error examination. There is a large pool of granular-fluid interaction scenarios for future application of this work. For expanded analysis of flow through fixed beds, this work can be applied to beds in columns of different diameters and of different geometry to determine how the solution trend changes with these parameters. Application of this work to beds of binary-sized particles would add another dimension of complexity as well. Outside of the simple fixed bed applications, the effect of grid size on the simulation results for fluidized beds is very important since the grid size can dictate phenomena such as bubbling or spouting, that are captured in the results. We plan on using the methods proposed in this work to analyze the errors present in the simulation of elutriation phenomena. Elutriation occurs in fluidized beds of granular mixtures containing large particle size variation.

The setup of grids for CFD-DEM applications is often arbitrary. The investigation of solution trends over refined grids of different types using the methods proposed in this study could lead to better grid design criteria.

The concept of an optimal grid size has been published repeatedly in the literature. The method outlined in this study was able to justify the choice of an optimal grid size for this application. Extension of this method to other applications could lead to a better understanding of the optimal grid size as a possible function of the particle diameter, column geometry and/or flow conditions. The next phase of this work includes analysis of cell shape on the resulting simulation error. Flow through a fixed particle bed in a square column will be simulation to analyze a variety of different meshing schemes. The square

column geometry will facilitate the analysis of solutions on a series of refined grids in which all cells are identical cubes. Simulation results employing meshes with identical average 3D grid size but different cell shapes will also be compared.

The recommendation emerging from this work is to begin establishing uniform reporting procedures across all granular-fluid flow simulations, and future work should consider expansion in all of these areas.

Appendix A

Appendix B

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