ABSTRACT

A two dimensional computational fluid dynamics (CFD) model has been developed to simulate the hydrodynamics of gas-solid flow in a high density circulating fluidized bed (HDCFB) riser using the commercial CFD software, Fluent. The Eulerian-Granular multiphase model was applied, which treats both phases as a continuum while the governing equations of mass and momentum conservation were solved for gas and solid phases. The kinetic theory of granular flow was used to provide the closure relations for the governing equations for the solid phase.

CFD modeling of the isothermal multiphase flow of air and fluid catalytic cracking (FCC) particles in a circulating fluidized bed (CFB) riser has been performed and compared to the experimental findings of particle volume fraction, particle axial velocity, and local particle solid flux profiles reported by J. Liu (Liu, PHD thesis, 2001 Department of Chemical and Biological Engineering, The University of British Colombia). The simulated profiles were overall in good qualitative agreement with the experiments, while similarly, the simulated particle axial velocities were in good quantitative and qualitative agreement with the experiments. However, due to the difficulties in modeling the solid segregation toward the wall accurately, the solid volume fraction was under predicted near the walls.

The effect of different drag models including Gidaspow, Arastoopour, and Syamlal and O'Brien drag models on modeling results was investigated. All the drag models predicted quite similar flow hydrodynamics; however, the Syamlal and O'Brien drag model, which was modified based on the minimum fluidization velocity of the applied FCC particles, indicated better predictions of the solid volume fraction profiles at the core area.

Different wall restitution coefficient values and solid slip conditions have been applied to study their effects on solid volume fraction distribution across the riser. While the wall restitution coefficient did not exhibit a significant effect on the riser hydrodynamics, the appropriate slip condition aided in predicting the solid segregation toward the wall. Using
the free solid slip condition resulted in a better agreement with the experimental data of the solid volume fraction distribution near the walls.

Finally, the model was evaluated comprehensively by comparing its predictions with experimental results reported for a circulating fluidized bed riser operating at a solid mass flux in the range of 94 to 550 kg/m²s and a superficial gas velocity in the range of 4 to 8 m/s. The model was capable of predicting the main gas-solid flow features in the HDCFB riser operating at a solid mass flux in the range of 254 to 455 kg/m²s. However, the model was incapable of accurately predicting the gas-solid flow behavior in a low density circulating fluidized bed riser with a solid mass flux of 94 kg/ m²s and risers operating in dense suspension up-flow regime with a solid mass flux of 550 kg/ m²s.
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**Symbols**

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<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tbody>
<tr>
<td>$A$</td>
<td>Area, m$^2$</td>
</tr>
<tr>
<td>$Ar$</td>
<td>Archimedes number</td>
</tr>
<tr>
<td>$C$</td>
<td>Courant number</td>
</tr>
<tr>
<td>$C_D$</td>
<td>Drag coefficient</td>
</tr>
<tr>
<td>$C_{fr}$</td>
<td>Coefficient of friction</td>
</tr>
<tr>
<td>$d_i$</td>
<td>Diameter, m</td>
</tr>
<tr>
<td>$e_i$</td>
<td>Restitution coefficient</td>
</tr>
<tr>
<td>$F_i$</td>
<td>Force, N</td>
</tr>
<tr>
<td>$g$</td>
<td>Acceleration due to gravity, m/s$^2$</td>
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<tr>
<td>$g_{0,i}$</td>
<td>Radial distribution coefficient,</td>
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<tr>
<td>$G_s$</td>
<td>Solid mass flux, kg/m$^2$s</td>
</tr>
<tr>
<td>$H$</td>
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<tr>
<td>$\bar{I}$</td>
<td>Stress tensor</td>
</tr>
<tr>
<td>$I_{2D}$</td>
<td>Second invariant of the deviatoric stress tensor</td>
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<tr>
<td>$i, j, l$</td>
<td>Directions</td>
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<td>$k$</td>
<td>Turbulent kinetic energy, kg/s$^3$m</td>
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<tr>
<td>$K_i$</td>
<td>Momentum Interphase exchange coefficient</td>
</tr>
<tr>
<td>$k_{\Theta_s}$</td>
<td>Diffusion coefficient for granular energy, kg/s m</td>
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<td>-------------</td>
</tr>
<tr>
<td>$S_{i,j}$</td>
<td>Mean rate of strain tensor, 1/s</td>
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<td>$v_i$</td>
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<td>Height in riser measured from inlet, m</td>
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**Greek letters**

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<tr>
<td>$\alpha_i$</td>
<td>Volume fraction</td>
</tr>
<tr>
<td>$\varepsilon_i$</td>
<td>Dissipation of turbulent kinetic energy, kg/(s$^3$m)</td>
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<tr>
<td>$\gamma_{\text{cm}}$</td>
<td>Collision dissipation of energy, kg/(s$^3$m)</td>
</tr>
<tr>
<td>$\eta_i$</td>
<td>Effectiveness factor</td>
</tr>
<tr>
<td>$\Theta_i$</td>
<td>Granular temperature, m$^2$/s$^2$</td>
</tr>
<tr>
<td>$\lambda_i$</td>
<td>Bulk viscosity, kg/s m</td>
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<tr>
<td>$\mu_i$</td>
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<tr>
<td>$\nu_i$</td>
<td>Kinematic viscosity, m$^2$/s</td>
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<tr>
<td>$\pi$</td>
<td>Constant pi (3.14159)</td>
</tr>
<tr>
<td>$\delta$</td>
<td>Delta function, units vary</td>
</tr>
<tr>
<td>$\rho_i$</td>
<td>Density, kg/m$^3$</td>
</tr>
<tr>
<td>$\bar{\tau}_i$</td>
<td>Stress tensor, Pa</td>
</tr>
<tr>
<td>$\phi$</td>
<td>Angle of internal friction, °</td>
</tr>
<tr>
<td>$\phi_{\text{gr}}$</td>
<td>Transfer rate of kinetic energy, kg/s$^3$m</td>
</tr>
<tr>
<td>$\sigma_{\text{gr}}$</td>
<td>Dispersion Prandtl number</td>
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**Others**

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<tr>
<td>$\partial,d$</td>
<td>Differential operator</td>
</tr>
<tr>
<td>$\nabla$</td>
<td>Nabla operator, 1/m</td>
</tr>
<tr>
<td>$\nabla$</td>
<td>Change in variable</td>
</tr>
</tbody>
</table>
### Subscripts

- \( b \): Bulk
- \( dr \): Drift
- \( g \): Gas
- \( i \): General index
- \( \text{max} \): Maximum
- \( mf \): Minimum fluidization
- \( \text{min} \): Minimum
- \( p \): Particles
- \( s \): Solids
- \( t \): Terminal (e.g., \( v_t \) is the terminal velocity)
- \( t \): Turbulent
- \( \tau \): Stress tensor
- \( q \): Phase
- \( w \): wall

### Abbreviations

- 2-D: Two dimensional
- 3-D: Three dimensional
- BASF: Baddish Aniline and Soda-Fabric
- DEM: Discrete element method
- CFB: Circulating fluidized bed
- CFD: Computational fluid dynamics
- DNS: Direct numerical simulation
- DSU: Dense suspension up-flow
- E-E: Eulerian-Eulerian
- E-L: Eulerian-Lagrangian
- FCC: Fluid catalytic cracking
<table>
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<tr>
<th>Fluent</th>
<th>CFD software written and distributed by Fluent Inc</th>
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<tr>
<td>HDCFB</td>
<td>High density circulating fluidized bed</td>
</tr>
<tr>
<td>MCC</td>
<td>Mitsubishi Chemical Corporation</td>
</tr>
<tr>
<td>NSERC</td>
<td>Natural Sciences and Engineering Research Council of Canada</td>
</tr>
<tr>
<td>VOF</td>
<td>Volume of fluid</td>
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</tbody>
</table>
ACKNOWLEDGMENTS

I wish to express my appreciation to the following people who in various ways assisted me in this work, as their continuous courage and support helped me confront the difficulties that I encountered over the last two years.

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CHAPTER 1

1. INTRODUCTION

The increase and diversity in multiphase applications stress the need for the development of more efficient and accurate experimental techniques, realistic simulations, and other research and design tools. Circulating fluidized bed (CFB) is one such application which is used widely for various industrial purposes including cracking, drying, catalyst regeneration, power generation, and combustion. The widespread applications of CFB are basically due to its features, including rapid mixing between the phases, the high heat and mass transfer, the ability of high gas throughputs, controllable residence time of particles, and finally, temperature uniformity (an absence of hot spots) [1,2].

CFB risers exhibit special gas-solid flow hydrodynamics. The flow along the riser has a core-annular structure. The solid mainly accumulates and moves slowly downward at the walls, while dilute solid phase moves rapidly upward in the core of the riser. Such variations in radial solid distribution and particle flow direction and velocity make the CFB systems more complex to understand. A combination of theoretical modeling and
experimental analysis helps describe the gas-solid flow in risers more precisely. Many researchers have investigated CFB extensively through experimental studies and/or theoretical modeling. Among those, Gidaspow [3,4] and Arastoopour [5,6] have focused in examining CFB system experimentally as well as theoretically through computational fluid dynamics (CFD). However, there are others who have focused on developing realistic modeling tools for such complex systems such as researchers Syamlal and O'Brien [7,8]. As well, there is a remarkable collaboration between industry and academia in this field; for instance, the Fluidization Research Centre (FRC), was established at the University of British Columbia in 1997 with funding provided by the Mitsubishi Chemical Corporation (MCC), the Natural Sciences and Engineering Research Council of Canada (NSERC), and a number of other governmental and industrial sponsors.

1.1 The Need For Further Studies

Computational fluid dynamics (CFD) is the use of computer modeling to simulate hydrodynamics and other related parameters, heat transfers, and chemical reactions, for single and multiphase systems. CFD models possess a promising future and are expected to make valuable contributions in predicting the behavior of CFB systems. However, the available multiphase models lack in comprehensive experimental validations and are implicitly designed for specific operating conditions. At present, there are no systematic strategies available to make appropriate selection of models (e.g. laminar versus turbulence) and models parameters (e.g. values of restitution coefficient, specularity coefficient, and interphase drag coefficient) to simulate gas-solid flow in industrial risers.
Several researchers, such as Ranade [9] and Grace et al. [2] have discussed the need for further CFD development to perform more reliable modeling of CFB hydrodynamics.

Although, most of the industrial CFB reactors are operated with very high solid flux which has the potential to reach 1200 kg/m$^2$s [10], most of the modeling studies of CFB risers were carried out for systems operating with relatively low solid mass flux. To the author’s knowledge, the most severe operating condition that has been modeled for a high density circulating fluidized bed (HDCFB) was with 489 kg/m$^3$s solid mass flux and 5.2 m/s superficial gas velocity [6]. According to Grace [11], a CFB riser operating with a relatively high solid circulation rate (300-1000 kg/m$^3$s) and a high gas superficial velocity (6-10 m/s) has a different fluidization regime with more uniform radial solid distribution compared to risers operating in fast fluidization regime and an absence of net solid downward flow.

1.2 Research Objective

The objective of this work is as follows:

- To develop a 2-D CFD model which describes the hydrodynamics of a gas-solid flow in a HDCFB riser using a commercial CFD package (Fluent Inc., FLUENT 6.2).
- To compare the CFD predictions of HDCFB hydrodynamics by applying laminar and turbulence models.
- To evaluate the sensitivity of modeling predictions to different modeling parameters. This evaluation includes the following parameters:
CHAPTER 1: Introduction

- Gas-solid interphase exchange coefficient by applying different drag models including Gidaspow, Arastoopour, and Syamlal and O'Brien drag laws.
- Particle-wall restitution coefficient by using different values of 0.9, 0.95, and 0.99.
- Particle tangential slip conditions by assuming no-slip, free-slip, and relatively high slip conditions.

- To evaluate the CFD models by comparing the predictions with experimental results from the literature for a broad range of operating conditions.

1.3 Thesis Structure

In Chapter 2, a general background and review of what have been performed lately in fluidization and multiphase modeling are presented. Some topics such as fluidization regimes and classification of multiphase modeling, and turbulence modeling are presented in more detail due to their significance in the current study.

Chapter 3 describes the development of a CFD gas-solid multiphase model of a HDCFB riser, where modeling procedure and a comparison of different models and model parameters are presented in detail. Finally, model performance is discussed and evaluated by comparing the predictions with the experimental results.

In Chapter 4, the CFD model is evaluated by applying different operating conditions under different fluidizations regimes.
CHAPTER 1: Introduction

In Chapter 5, the conclusions of this work and the recommendations for future explorations in the area of HDCFB CFD modeling are presented.
1.4 Literature Cited

CHAPTER 2

2 LITERATURE REVIEW

2.1 Fluidization

Fluidization is commonly defined as the operation by which fine solids are transformed into a fluid-like state through contact with a gas or liquid [1]. Fluidized beds are known for their high heat and mass transfer coefficients, due to the high surface area-to-volume ratio of fine particles. Fluidized beds are utilized in a wide variety of industrial processes such as reaction, drying, mixing, granulation, coating, heating, and cooling.

2.1.1 Fluidization Developments

The history of fluidization began in 1922 with Winkler’s patent of a fluidized bed process for coal gasification which was used for the production of synthesis gas. A period of 4 years witnessed the first lab-scale work to realize the process on the industrial scale in a fluidized bed reactor with a bed area of 12 m² and a total height of 11 m [2]. Compared to modern technologies, the Winkler gas producer is inefficient because of its high oxygen consumption and its large carbon loss by entrainment. With the increased use of
petroleum materials throughout the world, Winkler’s generators have gradually been replaced by generators that use petroleum feed-stocks.

Despite Winkler’s gas gasification process, fluidization was not particularly popular in the industry until 1942. There were large demands for the aviation fuel during World War-II, which could not be met by regular oil refining processes. A new fluidization process known as a fluid catalytic cracking (FCC) was developed by the Standard Oil Development Company (currently Exxon) in cooperation with M.W Kellogg Company and the Standard Oil Development Company of India (currently Amoco) [1] to crack the heavy oil and produce a greater amount of aviation fuels. The first unit was built at Exxon’s Rough Refinery with a capacity of 13,000 barrels/day. Successive modifications led to the ongoing construction of units which exceeded 100,000 barrels/day with further design improvements.

Following the fluid catalytic cracking process, several fluidization processes have been developed, e.g. Fluo-Solid system for roasting Sulfide ores and another unit for drying powdery material by the Dorr-Oliver Company in 1947 and 1984, respectively, and the fluidized bed roaster by the German company, Baddish Aniline and Soda-Fabric (BASF), in 1950 [1]. Following these advancements, many researchers became interested in the subject of fluidization with the fluidization community being gradually formed, where the first international conferences were held at Eindhoven in 1967 [3] and in 1976 at Asilomar [4]. Since then fluidization processes have gained in popularity and received greater attention for a wide range of chemical and physical operations.
2.1.2 Fluidization Regimes

Generally liquid-solid and gas-solid fluidization systems possess a multitude of characteristics in common but they behave quite differently. For example, the increase in flow rate above minimum fluidization usually results in a smooth expansion of the liquid-solid bed. However, for the gas-solid systems an increase of the flow rate beyond minimum fluidization results in large instabilities with bubbling and channeling of gas observed [1]. On the other hand, solids with different particle characteristics exhibit different fluidization behaviors. According to Geldart [5], powders can be classified into four groups \(A\), \(B\), \(C\), and \(D\) based on their mean size, density, and their fluidization properties. Groups \(A\), \(B\), and \(D\) follow the general fluidization regimes, while Group \(C\) powders are highly cohesive and hence cannot be subjected to normal fluidization. This section discusses the fluidization regimes in gas-solid systems with the chosen Geldart group \(A\) particles representing the conditions used for this study.

When gas is introduced at the bottom of a bed containing solid particles, at a very low flow rate, the gas passes through the voids between the stationary particles without moving the particles, (Figure 2.1). This is termed a fixed bed regime because the bed does not expand. In increasing the superficial gas velocity, \(U_s\), the voids between particles become larger and particles start moving and oscillating until they become totally suspended. At this point the drag exerted on the particles by an upward flowing gas balances the weight of the particles making the solid particles suspended. The superficial gas velocity at which this occurs is called the minimum fluidization velocity, \(U_{mf}\).
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With an increase of the superficial gas velocity, more fluidization regimes can be observed: namely, bubbling, slugging, turbulent, and fast fluidization. With an increase of the flow rate beyond minimum fluidization, large instabilities with bubbling and channeling of gas are observed forming the bubbling fluidization regime. As the bubbles rise in the bed they coalesce and grow while particles flow down the wall around the rising void of gas creating what is known as a slugging regime. By increasing a sufficiently high gas flow rate, the terminal velocity of the solid is exceeded and the solid entrainment becomes noticeable, thus instead of the creation of bubbles, a turbulent motion of solid clusters and void of gas are observed forming a turbulent fluidized bed. With further increase of the gas flow rate, solid entrainment becomes more significant and unless the entrained solids are replaced continuously the bed empties rapidly. This regime is known as fast fluidization.

2.1.3 Circulating Fluidized Bed

CFB is often used to maintain continuous operation for gas-solid fast fluidization systems. Solid particles are separated from the gas through a cyclone and recycled to the bottom of the column. As shown in Figure 2.2, CFB flow patterns depend on both the gas superficial velocity, $U_g$, and the solid circulation rate, $G_s$. If the superficial gas velocity is sufficiently high at a fixed low solid circulation rate, all particles are conveyed up the column with no accumulation at the bottom. This represents the pneumatic conveying regime. Grace et al. [6,7] has shown that with an increasing solid circulation rate above 300 kg/m²s at a fixed high gas velocity 6-10 m/s, a new flow regime called the dense suspension up flow (DSU) regime transpires. DSU offers a greater uniformity in radial
solid distribution compared to the fast fluidization regime and an absence of net solid downward flow near the walls. Although the DSU regime has only recently been identified as a new fluidization regime, it has been applied extensively in fluid catalytic cracking for many years.

In the past two decades, due to the practical limitations of academic laboratories, CFB risers have been investigated extensively at relatively low solid fluxes (<100 kg/m²s) and overall volumetric solid concentrations less than approximately 10% [8]. Since 1993, a series of studies on high density circulating fluidized bed (HDCFB) have recently been undertaken at the University of British Columbia with the development of advanced experimental equipments and techniques such as the dual loop circulating fluidized bed developed by Grace et al. [6] and the use of dual function optical probes developed by Liu et al. [9,10]. The hydrodynamics of HDCFB have been measured at more severe operating conditions with solid fluxes up to 600 kg/m²s, overall solid fractions of up to 20-25 % of the riser, and superficial gas velocities up to 9 m/s. It has been reported that the downward velocities near the walls diminish or even disappear, signifying a transition to the new flow regime, DSU [6]. This means that the core-annular structure, which characterizes the CFB multiphase flow operating in a fast fluidization regime, does not exist in the DSU regime.
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2.2 Computational Fluid Dynamics

2.2.1 Modeling Hydrodynamics of CFB Risers

Harris and Davidson [11] categorized the models to compute gas-solid multiphase flow in CFB risers into three main categories used by many authors to classify the CFB modeling techniques of Gómez and Milioli [12], Koksal [13], and Torres [14], for example.

Class I models predict only the axial behavior of solid density in the riser without considering the radial distribution. Pressure gradients and empirical correlations are used to predict the axial variations (Kunii and Levenspiel [15], and Li and Kwauk [16]). However, solids segregation exists in the CFB risers and are characterized by a core-annular flow that cannot be computed by such models. Class II models predict the radial variation of the density of solids and the high average slipping velocities, accounting for two or more regions of different flow characteristics (such as the core-annular flow) as described by Pugsley [17], and Berruti et al. [18]. Both classes of the models require experimental measurements for the specific system to be modeled in order to define the empirical correlations, which essentially makes them non-predictive and unable to be generalized for different systems. Despite the fact that these two classes display good agreement with the experimental data, there is a need for more general models that can function independently.

Class III models are much more complicated than the previous two classes, are more general, can be applied for more complex geometries, and account for both the radial and
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the axial variations. These models are based on the fundamental conservation equations of fluid dynamics; however, they require closure laws for these equations which are achieved through empirical and semi-empirical information obtained for different systems. Because of the applicability of class III models, most recent works such as Sinclair and Jackson [19], Benyahia et al. [20], and Neri and Gidaspow [21] used this class of models.

2.2.2 Multiphase Modeling Approaches (class III)

There are several numerical approaches to model the multiphase flows using the fundamental conservation equations of fluid dynamics. The main three approaches and the most popular ones for modeling multiphase flows are the volume of fluid (VOF), the Eulerian-Eulerian (E-E), and the Eulerian-Lagrangian (E-L) models [22]. The Direct numerical simulation (DNS) [23] and the discrete element method (DEM) [24] are much less popular from an engineering and research point of view. These models demand a very fine meshing which results in massive computational costs. This fine meshing allows for the calculation of many values, such as the interaction forces between particles, instead of using empirical approximation.

The VOF model is a surface tracking technique designed for two or more immiscible fluids where the position of the interface between the fluids is of interest such as the motion of large bubbles in a liquid. In the VOF model, a single set of momentum equations is shared by the fluids, and the volume fraction of each of the fluids in each computational cell is tracked throughout the domain [25]. While this approach is limited
to modeling the motion of only a few dispersed phase particles, it can provide valuable information to develop appropriate closure models for E-L and E-E approaches [22].

The Eulerian-Lagrangian approach, known also as discrete phase model, treats the fluid as a continuum by solving the time-averaged Navier-Stokes equations, while Newtonian equations of motion are solved for each individual particle, bubbles, or droplets of the dispersed phase. The dispersed phases can also exchange momentum, mass, and energy with the fluid phase. The E-L approach is applied to multiphase flows for dilute systems where a continuum model for the particle is not appropriate. This model is appropriate for the modeling of spray dryers, coal and liquid fuel combustion, but inappropriate for the modeling of fluidized beds, or any application where the volume fraction of the second phase is not negligible.

In CFD, the Eulerian-Eulerian approach has become more popular for simulating gas or liquid and solid multiphase systems, treating both phases as an interpenetrating continuum by solving a set of conservation equations for each phase. Closure laws, needed to define some fluid parameters for the solid phase such as viscosity and pressure, are achieved through constitutive equations which are obtained by the application of the kinetic theory of granular flow. This theory is based on the kinetic theory of gases which was defined by Chapman and Cowling in 1970 [26]. Kinetic theory of gases is the study of the microscopic behavior of molecules and their interactions. For dense systems, the motion of the particles forming the solid phase is comparable to the motion of the gas molecules forming the gas phase, but at a larger scale. Therefore, one may construct an
analogy between a random motion of particles and a thermal motion of gas molecules by introducing the term, granular temperature, or $\Theta$. Since Sinclair and Jackson [18] applied kinetic theory of granular flow to compute gas-solid hydrodynamics of a fully developed gas-solid flow in a pipe in 1989, it has become a very common application for most of the fluid-solid flows in dilute to dense bed regimes (e.g. [20,21]).

Ibsen et al. [27] evaluated the numerical prediction of multiphase E-E and E-L models. The numerical predictions from the discrete particle model were found to be in better agreement with experimental findings, but the E-E model was by far the most efficient. It took more than 100 times longer for the E-L model to obtain the modeling results when the two simulations were run on the same computer.

2.2.3 Turbulence Modeling of CFB

Flows can be classified into two main types according to their Reynolds number, laminar, and turbulent. For turbulent flow, the time-averaged continuity and momentum equations are presented by the following equations, respectively.

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho \bar{u}_i) = 0 \tag{2.1}
\]

\[
\frac{\partial}{\partial t} (\rho \bar{u}_i) + \frac{\partial}{\partial x_j} (\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \left[ \mu \frac{\partial \bar{u}_i}{\partial x_i} + \frac{\partial \bar{u}_j}{\partial x_j} \right] - 2 \delta_{ij} \frac{\partial \bar{u}_i}{\partial x_j}\tag{2.2}
\]

\[
+ \frac{\partial}{\partial x_j} (-\rho u'_i u'_j)
\]
where, $\bar{u}$ is the time-averaged velocity, and $u'$ is the fluctuating velocity. An additional term $\overline{u'u_j}$ appears on the right hand side of the time averaged momentum equations. This term, Reynolds stress, exhibits the form of stress. A closure model is required for Equation 2.2 because an exact analytical solution for the Reynolds stress is impossible to obtain.

A variety of turbulence models are available, with $k-\varepsilon$ models being commonly used due to their simplicity and reasonable accuracy for a wide range of turbulent flows. These models solve the averaged Navier-Stokes equations by the introduction of two additional transport equations, the turbulent kinetic energy, $k$, and its dissipation rate, $\varepsilon$. Studies of the Standard $k-\varepsilon$ model began with Harlow and Nakayama [28], who developed a modeled form of the exact transport equation for the energy dissipation rate. Jones and Launder [29] analyzed the transport equation for the energy dissipation rate with the transport equation for turbulent kinetic energy and empirical constants to further develop the standard $k-\varepsilon$ model.

The turbulence in the gas phase of a gas-particle flow is similar to the turbulence of a single phase, but is highly influenced by the presence of particles [30]. Berker and Tulig [31] are considered to be the first to introduce the turbulence model into a multiphase model. However, their model accounts only for gas turbulence and neglects the particle turbulence. Zhou and Huang [32] developed the $k-\varepsilon-k_p$ model simulating gas-particle flow by accounting for both phases turbulences. Zheng et al. [33] used the $k-\varepsilon-k_p-\varepsilon_p-k_p-\Theta$ model, which accounts for the two phase turbulence and the
particle-particle collisions by the introduction of kinetic energy dissipation rate of solid phase and kinetic theory of granular flow, to study gas-solid flow in a riser. The predicted results showed satisfactory agreements with the experimental data. The detailed analysis indicates that the interaction between the turbulence of gas and that of particles was a crucial factor in influencing the predicted results.
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Fig. 2.1: Fluidization regimes.
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Fig. 2.2: Pneumatic conveying and DSU regimes.
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2.3 Literature Cited

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CHAPTER 3

3 COMPUTATIONAL FLUID DYNAMICS OF HIGH DENSITY CIRCULATING FLUIDIZED BED RISER: STUDY OF MODELING PARAMETERS

3.1 Introduction

When the fluidized bed is operated above the terminal velocity of the particles, they are carried out of the bed. The particles can be separated from the fluid by the use of cyclones and recycled to the bed. This system is termed a Circulating Fluidized Bed (CFB). The part of the system where the carryover of solids transpires is normally referred to as the riser.

CFB is widely used for various industrial applications including cracking, drying, catalyst regeneration, power generation, and combustion [1]. The increase and diversity in CFB applications demand the need for the development of more efficient experimental techniques, realistic simulations, and other research and design tools. In spite of many CFB applications, the complexity of the interaction between phases in the risers presents a tangible challenge to the improvement and understanding of these systems. The CFB
design is notably complex in terms of scaling-up difficulties, because of the high sensitivity of the flow to scale and operational conditions [2]. The optimum design and scale-up of CFB risers require a fundamental understanding of the mixing patterns of phases including the variations on solid distributions, the continuous formation and dissipation of clusters, and the solid down-flows.

In the past two decades, many researchers have shown great potential for employing numerical simulation to study CFB hydrodynamics. With the development of high performance computers and advances in numerical techniques and algorithms, computational fluid dynamics (CFD) tools are increasingly gaining popularity. Some information such as turbulence parameters, which cannot be obtained or are hard to obtain in laboratory conditions, is easily estimated using CFD tools [3]. In addition, CFD models provide a more detailed data profile as a function of space and time without interfering or disturbing the flow by internal probes [3]. Although modeling tools help explain the fluid behavior more accurately, experimental studies are required to evaluate any multiphase CFD model. Particle velocities and concentrations are particularly essential to determine different fluidization properties such as suspension densities, local solid flux, and solid effective viscosities. Until 1987, dense flow hydrodynamic experiments measured either only the particle velocities or the particle concentrations [4]. The Bader et al. [5] study appears to be the first in which both the particle velocities and the particle concentrations were determined for the riser flow. Since then, modelers been able to compare and evaluate their theoretical models with experimental studies in detail.
Currently, the Eulerian-Eulerian (two-fluid) model with kinetic theory of granular flow is the most applicable approach to compute gas-solid flow in a CFB (e.g. [6-11]). This model is particularly appropriate when the particle loading is relatively high and can be applied with reasonable computation effort. In the two-fluid model, the particles are treated as a continuum as in the gas phase. Thus, there are two interpenetrating phases (gas and solid) where each phase is characterized by its own conservation equation of motion. The interactions between the two phases are expressed as additional source terms added to the conservation equations. The kinetic theory of granular flow is used to define the fluid properties of the solid phase through constitutive equations. Detailed discussion on the development of granular flow models is provided by Gidaspow [12].

Although CFD models have a promising future and are anticipated to make valuable contributions to predicting the performance of CFB reactors, currently, there are no systematic guidelines available to make appropriate selection of models and model parameters (such as laminar versus turbulent, values of restitution coefficients, specularity coefficient, and interphase drag coefficients) to simulate gas solid-flow in industrial risers [3]. Various authors have utilized different models, laminar or turbulence, with kinetic theory of granular flow for modeling the hydrodynamics of gas-solid multiphase risers. In some cases, satisfactory agreements with experimental data have been reported in applying both the laminar viscous model (e.g. [6-8]) and the $k - \varepsilon$ turbulence model (e.g. [11]). However, none of these studies have compared the two model performances for the same systems. In general, multiphase flows in risers are very turbulent displaying high Reynolds number, which could mean taking into account the
time averaged turbulent behavior and the turbulent interaction between phases make simulation predictions more realistic. However, unless an appropriate turbulence model with the correct empirical constants and closures is chosen, the model predictions may be less consistent than the laminar model. Zheng et al. [10] compared three different turbulence models with different closures; two models which consider the turbulence effect of the two phases and one which ignores particles turbulence. The model which ignores the particles turbulence showed by far the greatest inconsistency predictions with the experimental data. Although the other two models demonstrated better predictions, only one of them showed reasonably good agreement with the experimental data. Therefore, more attention should be paid to select the most appropriate turbulence model with the correct empirical constants and closures of the transfer and dissipation of turbulent energy between gas and solids.

In spite of many CFB modeling studies that have been performed in the past two decades, there are some areas that have not been predicted precisely. In CFB risers, solids segregate towards the walls which can generate a down flow of some material under certain operating conditions. Most of the models available today are not able to describe this segregation of solids accurately, and therefore underestimate the solids concentration at the walls [8]. Therefore, more accurate definitions of most gas-solid interaction parameters are required in order to render more reliable CFB hydrodynamics modeling. Several researchers such as Ranade [3] and Grace et al. [1] have discussed the need for further development to understand and predict the behavior of the CFB systems.
CHAPTER 3: CFD of HDCFB Riser: Study of Modeling Parameters

The main objective of the current work is to develop a CFD model which will describe the hydrodynamics of a HDCFB using a commercial CFD package (Fluent Inc.). Different drag models including Gidaspow [13], Arastoopour [14], and Syamlal and O’Brien (modified based on the minimum fluidization velocity) [15], were examined to predict the most representative gas-solid interphase exchange coefficient. The solid behavior near the wall was studied closely by comparing the effect of different wall restitution coefficient values and slip conditions. The performance of two different viscous models, the laminar and the \( k-\varepsilon \) turbulence model with kinetic theory of granular flow was evaluated by comparing their predictions with experimental results from the literature.

3.2 Experimental Setup

The experimental studies on the hydrodynamics of HDCFB by Liu et al. [16,17,18] were used to evaluate the simulation results. The experimental apparatus, shown schematically in Figure 1, and the measurement techniques are briefly described as follows [16]:

Suspended particles in the first riser are directed to the first downcomer, from where they are fed into the second riser of a larger cross-sectional area. When the first riser is operated under high density conditions, the second riser tends to be much more dilute with a lower pressure drop and consequently lifts the solids from the first riser to a higher level, facilitating a taller downcomer. The bottom of the second downcomer possesses the highest pressure in the whole loop, sufficient to push enough particles through the J-valve and up the first riser.
The particles used throughout this experiment were FCC particles of 70 \( \mu \text{m} \) mean diameter while the gas used was air. The hydrodynamic characteristics of the first riser with more emphasis at the 3.8m height measured from the inlet of the riser were studied under various operating conditions. A dual function optical prop was used to measure local particle volume fraction and local particle velocity simultaneously. This technique allows for predicting the local solid flux by integrating a multiplication of local particle volume fraction and local velocities over the riser cross section. Detailed discussions of the measurement techniques are provided elsewhere [18,19].

### 3.3 CFD Modeling

The governing and constitutive equations, the boundary and initial conditions, as well as the numerical procedure used in the CFD modeling are described as follows:

#### 3.3.1 Governing Equations

The model proposed to describe the gas-solid hydrodynamics in the riser section of the HDCFB is based on the Eulerian-Granular model of Fluent V6.2 [20], where different phases can be present at the same time in the same computational volume by the introduction of a new dependent variable, the volume fraction, \( \alpha_q \), of each phase, \( q \). Particles are assumed perfectly spherical and mono-sized, hence only one solid phase is considered with an average particle size.

The fundamental equations of mass and momentum conservation were solved for each phase (Table 3.1); and assumed an absence of mass transfer between the phases. The energy conservation equation was ignored as the flow is isothermal (cold flow...
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experiment). In addition to the mass and momentum conservation equations for the solid phase, a fluctuation kinetic energy equation, Equation 3.5, is also solved to account for the conservation of the fluctuation energy of solid particles, through the implementation of the kinetic theory of granular flow.

Several closure models have been proposed to define appropriate constitutive equations for binary and multi-phase flows based on the kinetic theory of granular flow. The closure model used in this work is described in Table 3.2. Equations 3.6-3.24 list the constitutive equations needed to close the solid phase momentum conservation equation for phase stress tensor, $\bar{\mathbf{e}}$, solid pressure, $p_s$, and the momentum exchange between the solid and gas phases, $K_{pg}$. The momentum exchange is a function of virtual mass, lift, and drag force. Stock [21] has shown that for gas-particle flows with $\rho_s / \rho_g \approx 1000$ the virtual mass effect is insignificant and can be neglected. On the other hand, the lift force will be more significant for larger particles, but since the particle size used in this study is relatively small (70 μm), the inclusion of lift force was neglected. Therefore, the gas-solid momentum exchange coefficient is assumed to only include the drag contribution.

Several drag models exist for the gas-solid interphase exchange coefficient. In this study, the performance of different drag models, including Gidaspow [13], Arastoopour [14], and Syamlal and O'Brien drag models was examined. The Syamlal and O'Brien drag model was modified based on the minimum fluidization velocity of the particles. The procedure of modifying the drag law was provided by Syamlal and O'Brien [15]. Equations 3.25-3.27 list additional constitutive equations required to close the fluctuation
energy equation for the thermal diffusion coefficient, \( k_{\text{eq}} \), the collision dissipation energy, \( \gamma_{\text{eq}} \), and the transfer of kinetic energy, \( \phi_{\text{eq}} \), between the gas and solid phases.

Tables 3.1 and 3.2 list the governing equations and their constitutive equations for a laminar model without considering the turbulent behavior. To account for the interactions of turbulence between the gas and solid phase, the conservation equation of motion should be averaged over a period of time that is longer than the period of the longest fluctuations. A variety of turbulence models are available; however, the \( k - \varepsilon \) models are commonly used due to their simplicity and reasonable accuracy for a wide range of turbulent flows. The single phase \( k - \varepsilon \) model was modified for the continuous phase by the introduction of the interphase turbulent momentum transfer term. The predictions for turbulent quantities for the dispersed phases were given in terms of the mean characteristics of the primary phase, the ratio of the eddy-particle interaction time, and the particle relaxation time. The turbulence model used in the current work is summarized by Benyahia et al. [22].

3.3.2 Boundary and Initial Conditions

The schematic diagram of the riser with the boundary and initial conditions used in this work is presented in Figure 3.2. At the inlet, all velocities and volume fractions of both phases were specified. The average solid velocity at the inlet is calculated from the following relation based on the given solid mass flux:

\[
\frac{u_{p,m}}{G_{\text{riser}}} = \frac{\rho_s A_{\text{riser}}}{\rho_s \alpha_s A_{\text{inlet}}} \quad \text{(3.28)}
\]
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This equation produces an average solid velocity of 1.3 m/s at the inlet for a volume fraction of 0.55 and a flux of 455 kg/m²s. At the outlet, the pressure was specified (atmospheric). At the wall, the gas tangential and normal velocities were set to zero (no-slip condition) while the normal velocity of the particles was also set at zero. The following boundary equations, developed by Johnson and Jackson [23], were applied for the tangential velocity and granular temperature of the solid phase at the wall:

$$u_{s,w} = -B \frac{\partial u_{s,w}}{\partial n}$$

(3.29)

$$B = \frac{6\alpha_s \mu_s}{\sqrt{3} \Theta \pi \rho_s \alpha_s g_{n,w}}$$

(3.30)

where the specularity coefficient, $\phi$, is specifically used in multiphase with granular flow to express the slip coefficient, $B$. The specularity coefficient is a measure of the fraction of collisions which transfer momentum to the wall and its value ranges between zero and unity.

The granular temperature at walls, $\Theta_w$, is obtained in term of the collisional dissipation at the wall, $\gamma_w$, as:

$$\Theta_w = -C_1 \frac{\partial \Theta_w}{\partial n} + C_2$$

(3.31)

$$C_1 = \frac{k \Theta_x}{\gamma_w} ; \quad C_2 = \frac{\sqrt{3} \pi \rho_s \alpha_s u_{s,\text{slip}} g_{o,\Theta_x} \Theta_x^{3/2}}{6 \alpha_{s,\text{max}} \gamma_w}$$

(3.32)

where $\gamma_w$ is expressed in terms of wall restitution coefficient $e_w$, as:

$$\gamma_w = \frac{\sqrt{3} \pi (1 - e_w^2) \alpha_s \rho_s g_{o,\Theta_x} \Theta_x^{3/2}}{4 \alpha_{s,\text{max}}}$$

(3.33)

In order to assess the effect of boundary conditions at the wall, different cases with different specularity and wall restitution values were investigated. The dimensions of the
main riser, gas and particle properties, and other modeling parameter are presented in Table 3.3.

3.3.3 Numerical Procedure

The governing equations are solved using the finite volume method, where the partial differential equations are defined in volume integral form. The second order upwind discretization schemes were used to solve the convection terms. The Phase Coupled SIMPLE (PCSIMPLE) algorithm by Vasquez and Ivanov [24], which is an extension of the SIMPLE algorithm of multiphase flows [25], was used for the pressure-velocity coupling and correction.

The riser was simulated in a two dimensional domain (2-D) as shown in Figure 3.2. The dimensions of the domain in radial and axial directions were similar to those of the actual riser in experimental apparatus, 0.076 m and 6.1 m, respectively. The total number of cells used to construct the grid was set at 21,560 (75 x 308). In the radial direction, the grid spacing was distributed non-uniformly; more cells were placed closer to the wall to capture the complex flow behavior in this region. However, uniform grid spacing was used in the axial direction except at the outlet region where the grid spacing is decreased to stress the exit effect. The maximum cell sizes are 0.0017 m in the radial and 0.05 m in the axial direction.

A time step of $5 \times 10^{-4}$ s with 100 iterations per time step was used in the simulation to ensure numerical stability. During the first fifteen seconds, the solid density in the riser was increasing until quasi-steady-state conditions were reached for the integral outlet.
solid flux. Therefore, the time averaged distributions of flow variables were computed after reaching the steady state conditions; from 15 s to 37 s. A convergence criterion of $1 \times 10^{-4}$ was specified for the relative error between two successive iterations. The typical computational time for this simulation was 8-12 days on a 1.6 GHz workstation.

3.4 Results and Discussion

3.4.1 Inlet Investigation

The solid feeding system of the main riser consists of a J-valve equipped with a main air inlet, two secondary air ports, and a venture section (Figure 3.3). In this configuration, the particles descending from the downcomer are first aerated and accelerated through the J-valve and then move vertically upward as they converge with the main air flow. The objective of the venture section at the bottom of the main riser is to avoid particle blockage and to allow the gas and particles to mix more uniformly.

Since there were no experimental observations describing the gas-solid distribution at the inlet, the flow distribution was investigated numerically by modeling a 2-D combined geometry of the inlet section and the riser. Figure 3.4 shows particles volume fraction and axial particle velocity distributions throughout the inlet section (the riser was considered for a more accurate modeling results, but is not shown in the figure). Particles are dragged vertically toward the wall, which is expected considering the gas is entering the system vertically at a relatively high velocity ($\approx 11$ m/s) compared to the particles which meet the gas flow at a relatively low velocity ($< 2$ m/s).
Miller and Gidaspow [26] studied experimentally the gas-solid distributions for the inlet section of a CFB riser similar to the system simulated in this work but with the feeding of solid and gas occurring through an inner tube at the riser bottom. Several measurements were carried out at the inlet section, such as solid velocity, volume fraction, and granular temperature. Although the exact inlet conditions were difficult to measure due to their transient nature and, as a consequence, their low, the data provided evidence of some accumulation of solid at the inlet tube wall. The associated velocity was also lower than the core velocity. This inlet condition agreed with the predicted radial profile of solid volume fraction (Figure 3.5a) and axial particle velocity (Figure 3.5b) predicted by the current inlet section model. The particle volume fraction reaches a maximum value of 0.55 with a velocity as low as 2 m/s near the right wall.

Neri and Gidaspow [7] modeled the flow hydrodynamics in the same riser that was studied experimentally by Miller and Gidaspow [26] (mentioned above) using a uniform gas and solid distribution in the inner tube. Although the model predicted the most significant features of the two-phase flow riser hydrodynamics, a comparison between simulation results and experimental data at the middle cross section of the riser showed significant dissimilarities. The core solid concentration profile was flatter with a remarkable difference as low as one third of that measured experimental. The axial particle velocity at the center was twice as that of the experimental data. A uniform plug-flow feeding through the entire riser base was also implemented by some authors such as Samuelsberg and Hjertager [27,28]. This inlet condition was unable to properly represent the hydrodynamics at the lower section of the riser. The implementation of correct inlet
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conditions appears to be critical for a successful simulation of flow hydrodynamics. Both feed geometry and flow conditions through the inlet cross section can affect the flow pattern in the riser.

Given the system is actually three dimensional (3-D) with a cylindrical geometry, the gas flow will be surrounded by particles from more than one side. Therefore, to have an entrance zone flow distribution in 2-D simulation similar to that of a 3-D system, the velocity profiles in Figure 3.5 were divided equally into two sections to feed symmetrically through both sides of the riser as shown in Figure 3.2 (inlet). The exact experimental inlet configuration and conditions cannot be implemented unless a 3-D simulation is conducted in a more complex geometry. This requires a considerably high computational time with present workstation capabilities.

3.4.2 Grid Independency

To confirm that the CFD results are independent of the mesh size, simulations of the system with 50 x 200, 75 x 308, and 100 x 400 grids (radial x axial) were performed. As shown in Figure 3.6, the fine mesh case and medium mesh case predicted similar solid volume fraction distributions. This indicates that the medium mesh size (selected as a base case) is sufficiently fine for providing reasonably mesh independent results. In general, the continuous increase in mesh density may lead to slightly better results that are more grid-independent. However, the computational power currently available is still a significant restriction when using a finer mesh.
3.4.3 Parametric Study

Since there is no certainty of the appropriate model parameters such as the values of the restitution coefficient, specularity coefficient, and interphase drag coefficients, an investigation of the most appropriate model parameters for the riser were performed. Specularity coefficient, $\phi$, is used in multiphase granular flow to specify the shear condition at the walls. The specularity coefficient is a measure of the fraction of collisions which transfer momentum to wall and varies from zero (smooth walls) to one (rough walls). For specularity coefficient approaching zero, a free-slip boundary condition for the solids tangential velocity is obtained at the walls, while when approaching unity, a significant amount of momentum transfers. The particle–wall restitution coefficient, $e_w$, describes the amount of the dissipation by collisions of solids turbulent kinetic energy with the wall. A value of $e_w$ close to unity implies very low dissipation of granular energy at the wall.

Because of the difficulties associated with measuring the specularity coefficient, $\phi$, and the particle–wall restitution coefficient, $e_w$, for a given gas-particle flow system, different values were examined to select the best ones representing the system under investigation. Four different specularity coefficient values ($\phi = 1, 0.5, 0.1, \text{ and } 0$) and three different particle–wall restitution coefficient values ($e_w = 0.9, 0.95, \text{ and } 0.99$) were compared (Figures 3.7 and 3.8, respectively). Since a zero specularity coefficient can not be applied mathematically to calculate the slip coefficient ($\phi$ in the dominator of Equation 3.30), an equivalent zero shear condition at the wall is applied by Fluent to obtain the free-slip condition [20].
CHAPTER 3: CFD of HDCFB Riser: Study of Modeling Parameters

Using a free-slip boundary condition ($\phi = 0$), the solid volume fraction predictions were in better agreement with the experimental data, while the other values underestimated the solid volume fraction near the wall (Figure 3.7a). Benyahia et al. [22] and He and Simonin [29] have reported that a better agreement with the experimental data was achieved by using lower specularity coefficient values. It is likely because the higher the friction at the wall, the higher the turbulence level and the lower the predicted solids volume fraction. Thus, with a smaller specularity coefficient (less friction), a higher solids volume fraction near the wall is predicted which is in a better agreement with the experimental data. The specularity coefficient value produced less impact on the axial particle velocity (Figure 3.7b) except for the no-slip condition ($\phi = 1$).

Varying the wall restitution values did not affect model predictions significantly neither for solid volume fraction nor for axial particle velocity (Figures 3.8a and 3.8b, respectively). These results confirms observations by Neri and Gidaspow [7] and McKeen and Pugsley [30] that wall restitution coefficient plays only a minor role on a multiphase system with the Geldart A particles (FCC particles). Neri and Gidaspow [7] examined two wall restitution coefficients of 0.96 and 0.8 for CFB riser and reported that the wall restitution coefficient has some effect on the solid concentration near the wall, but its value is not critical for the overall definition of the flow pattern. Even a quite large variation of this parameter increased the solid concentration at the wall by only a small percentage and did not impact the dynamic behavior of the flow. On the other hand, Goldschmidt et al. [31] reported that varying this parameter resulted in a significant impact on bubbling bed hydrodynamics with the Geldart B particles.
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To calculate the gas-solid momentum interphase exchange coefficient, several drag models including Gidaspow, Arastoopour, and Syamlal and O'Brien were compared. The Syamlal and O'Brien drag model was modified based on the minimum fluidization condition of the FCC particles used in this study [15]. As presented in Figure 3.9, all the drag models examined predicted quite similar solid volume fraction and axial particle velocities. However, the Syamlal and O'Brien drag model showed a better prediction at the core area. This model is reported to provide a good description of the hydrodynamics of fluidized bed reactors with FCC particles of similar size [32].

Among the modeling parameters studied, the best agreement between the model predictions and experimental data were obtained by using free-slip boundary condition, modified Syamlal and O'Brien drag model, and \( e_w = 0.95 \). Therefore, these parameters were used for the full model analysis. In order to save time and reduce the computational effort a lower order of discretization (first order) with lower convergence precision \( (1 \times 10^{-3}) \) were used for the parametric study and mesh refinement test; while a higher order (second order) discretization and more precise convergence criterion \( (1 \times 10^{-4}) \) were used for the remainder of the study.

3.4.4 Comparison of Model Predictions and Experimental Results

Figures 3.10 and 3.11 reveal the transient behavior of solid volume fraction and the axial particle velocity for the middle section of the riser (3.2 m to 4.4 m) for the period of 0 s to 35 s from the beginning of the simulation. After 2.5 s, particles reach the middle section of the riser and as particles continue to move upward, the density of particles in the bed
increases until a statistically quasi-steady-state condition is reached after 15 s. Particles accumulate near the wall and form solid clusters (red colors in Figure 3.10). The size of these clusters increases until they become sufficiently heavy that they cannot be carried by the gas. Due to the gravity, particles moving downward (downward arrows in Figure 3.11) and solid circulation take place within the riser.

In order to compare simulation predictions with experimental results (averaged over 20-40 s), flow hydrodynamics were averaged over a time period of 15 s to 37 s. The integration of the solid mass flux over the riser outlet after 15 s of simulation was fluctuating ± 2.2% of that of the inlet, confirming satisfactory inlet/outlet mass balance simulated by the model and reaching steady state conditions. A comparison of laminar and turbulence model predictions with experimental results is presented in Figures 3.12a-d for radial and axial profiles of solid volume fraction, radial profile of solid mass flux, and radial profile of axial particle velocity, respectively. All the radial profiles of hydrodynamics are shown only for the right half of the riser at \(Z = 3.8\) m because there was no experimental data for the full cross section area. The full cross section profiles for the solid volume fraction and axial particle velocity were given in Figures 3.13a and b to show the model predictions for the other half of the riser. It is evident that the flow pattern is nearly axisymmetric despite the unsymmetrical configuration of the outlet geometry. This axisymmetrical behavior was shown experimentally for the same bed under different operating conditions by Liu [16].
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Given the time averaged profiles of solid volume fraction (Figure 3.12a) combined with the axial particle velocity (Figure 3.12d), it is evident that the flow along the riser has a core-annular structure, which characterizes the fast fluidization regime. The solid mainly accumulates and moves downward at the wall, while the dilute solid phase moves upward in the core of the riser. The main flow characteristics of the riser were well predicted by the modeling results. However, the solid volume fraction near the walls predicted by the model was found to be less than the experimental values had predicted (Figure 3.12a). This discrepancy, which has been reported by most of the CFB riser modelers (e.g. [6,7,33,34]), could be attributed to the simplifications used to reduce the computational difficulties of handling such complex and large systems. A 2-D representation of a 3-D system was modeled in this work; however, accurate model predictions are difficult to obtain unless the real 3-D geometry is modeled. In addition, the assumption of modeling particles with different sizes as monodispersed particles with an average particle diameter may contribute to this discrepancy. Zhang and Arastoopour [35] found that larger particles have more tendencies to accumulate near the wall than smaller ones. Therefore, assuming monodispersed particles could underestimate the effect of large particles accumulation near the wall, resulting in a lower solids concentration at the wall as predicted by the model.

Figure 3.12b shows the axial profile of solid volume fraction. It is clear that the model predictions agree qualitatively with the experimental data along the riser. However, the CFD model predicts higher solid concentration at the bottom section of the riser comparing to the experimental data. This could be due to the inaccurate modeling of the
inlet configuration. As explained earlier, the exact experimental inlet configuration and conditions cannot be implemented in the model unless the simulation of the complete 3-D geometry is conducted. However, this requires very high computational time with today’s workstation capabilities.

The time averaged radial solids flux was calculated by considering the particle velocity and volume fraction at each time step and averaging the resulted solid fluxes over the last 20 s when the quasi steady state condition was reached. Calculating the time averaged solid flux by considering the time averaged particle velocity and volume fraction, although seems acceptable, is not accurate because every particle velocity value should be considered with its volume fraction to obtain a representative solid mass flux at each point. The computational values of laminar and turbulence model of solid mass flux agreed well qualitatively with the experimental data (Figure 3.12c). The solids flux was at its maximum value near the center, and downflow solid particles were predicted near the walls. However, the CFD model over predicted the solid mass flux at the central region. Since the solid flux is a function of particle velocity and concentration, any difference between the model predictions and experimental data of either of these parameters results in a discrepancy of the computed solid flux.

Comparisons of the modeling results using the laminar and turbulence models are shown in Figures 3.12a-d. While laminar and turbulence models predicted similar axial particle velocities (Figure 3.12d), the turbulence model predicted higher solid volume fraction (Figure 3.12a) at the center (likely due to considering the turbulent fluctuation velocities...
in this model which enhance particle movements) and consequently higher solid flux (Figure 3.12c). This resulted in a lower solid volume fraction and solid flux predictions by the turbulence model over the remaining cross sectional area. Overall, the comparisons show that the laminar model predictions agreed better with the experimental data. In general, multiphase flows in risers are very turbulent exhibiting high Reynolds figures. Therefore, taking into account the time averaged turbulent behavior and the turbulent interaction between phases may make predictions more realistic. However, unless an appropriate turbulence model with the correct empirical constants and closures have been chosen, the model predictions may result in being less consistent than a laminar model. Therefore, more research is required to enhance the turbulence model performance by defining more appropriate closures and a constant that can best fit HDCFB systems.

3.5 Conclusion

A 2-D Eulerian-Granular model using Fluent V6.2 was able to simulate the hydrodynamics of a gas-solid HDCFB riser satisfactorily. The model was able to predict the core-annular flow structure which characterizes CFB risers operating in fast fluidization regimes. The model predicted a nearly axisymmetric flow pattern in the riser cross section, despite the unsymmetrical configuration of the outlet geometry. Using a free-slip boundary condition (equivalent to specularity coefficient equals zero, $\sigma = 0$), the solid concentration near the wall agreed better with the experimental data; while no-slip and relatively high slip boundary conditions underestimated solid concentration. Varying the wall restitution coefficient did not affect model predictions for the solid volume
fraction or for the axial particle velocity. Calculating the gas–solid momentum interphase exchange coefficient using the Gidaspow, Arastoopour, and Syamlal and O’Brien drag models was found to result in a similar prediction of the solid volume fraction and axial particle velocity profiles. However, the Syamlal and O’Brien drag model (modified based on the minimum fluidization condition) showed a better solid volume fraction prediction at the core area.
### Table 3.1: Governing equations

#### Gas phase

**Continuity**
\[
\frac{\partial}{\partial t}(\alpha_g \cdot \rho_g \cdot \vec{v}_g) + \nabla \cdot (\alpha_g \cdot \rho_g \cdot \vec{v}_g) = 0 \tag{3.1}
\]

**Momentum**
\[
\begin{align*}
\frac{\partial}{\partial t}(\alpha_g \cdot \rho_g \cdot \vec{v}_g) + \nabla \cdot (\alpha_g \cdot \rho_g \cdot \vec{v}_g^2) &= -\alpha_g \cdot \nabla p + \nabla \cdot \vec{F}_g + \alpha_g \cdot \rho_g \cdot \vec{g} + \alpha_g \cdot \rho_g \cdot K_{gs} \cdot (\vec{v}_g - \vec{v}_s) \\
\end{align*} \tag{3.2}
\]

#### Solid phase

**Continuity**
\[
\frac{\partial}{\partial t}(\alpha_s \cdot \rho_s \cdot \vec{v}_s) + \nabla \cdot (\alpha_s \cdot \rho_s \cdot \vec{v}_s) = 0 \tag{3.3}
\]

**Momentum**
\[
\begin{align*}
\frac{\partial}{\partial t}(\alpha_s \cdot \rho_s \cdot \vec{v}_s) + \nabla \cdot (\alpha_s \cdot \rho_s \cdot \vec{v}_s^2) &= -\alpha_s \cdot \nabla p - \nabla p_s \\
&+ \nabla \cdot \vec{F}_s + \alpha_s \cdot \rho_s \cdot \vec{g} + \alpha_s \cdot \rho_s \cdot (\vec{F}_{ex,s} + \vec{F}_{hyd,s} + \vec{F}_{vis,s}) \\
&+ K_{gs} \cdot (\vec{v}_g - \vec{v}_s) + \sum_{i,j=1}^{K_{sy}} (K_{sy} \cdot (\vec{v}_s - \vec{v}_g)) \\
\end{align*} \tag{3.4}
\]

**Kinetic fluctuation energy**
\[
\begin{align*}
\frac{3}{2} \left[ \frac{\partial}{\partial t}(\rho_s \cdot \alpha_s \cdot \Theta_s) + \nabla \cdot (\rho_s \cdot \alpha_s \cdot \vec{v}_s \cdot \Theta_s) \right] &= (-p_s \vec{I} + \vec{F}_s) \cdot \nabla \cdot \vec{v}_s \\
&+ \nabla \cdot (k_{sw} \cdot \nabla \cdot \Theta_s) - \gamma_{sw} + \phi_s \\
\end{align*} \tag{3.5}
\]
Table 3.2: Constitutive equations for momentum

<table>
<thead>
<tr>
<th>Phase</th>
<th>Enunciation</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>stress-strain</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>tensor</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( \bar{\mathbf{q}} = \alpha_q \cdot \mu_q \cdot (\nabla \cdot \bar{\mathbf{v}_q} + \nabla \cdot \bar{\mathbf{v}_q}') + \alpha_q \cdot \left( \lambda_q - \frac{2}{3} \cdot \mu_q \right) \cdot \nabla \cdot \bar{\mathbf{v}_q} )</td>
<td>(3.6)</td>
<td></td>
</tr>
</tbody>
</table>

| Solid shear       | \( \mu_s = \mu_{s,\text{col}} + \mu_{s,\text{kin}} + \mu_{s,\text{fr}} \)                     | (3.7)    |
|                   | \( \mu_{s,\text{col}} = \frac{4}{5} \cdot \alpha_s \cdot \rho_s \cdot d_s \cdot g_{\text{g,av}} \cdot (1 + e_{ss}) \cdot \left( \frac{\Theta_s}{\pi} \right)^{1/2} \) | (3.8)    |
|                   | \( \mu_{s,\text{kin}} = \frac{10 \cdot \rho_s \cdot d_s \cdot \sqrt{\Theta_s} \cdot \pi}{96 \cdot \alpha_s \cdot (1 + e_{ss}) \cdot g_{\text{g,av}}} \left[ 1 + \frac{4}{5} \cdot g_{\text{g,av}} \cdot \alpha_s \cdot (1 + e_{ss}) \right]^2 \) | (3.9)    |
|                   | \( \mu_{s,\text{fr}} = \frac{\rho_s \cdot \sin \phi}{2 \cdot \sqrt{I_{2D}}} \)                  | (3.10)   |

| Solid bulk viscosity | \( \lambda_s = \frac{4}{3} \cdot \alpha_s \cdot \rho_s \cdot d_s \cdot g_{\text{g,av}} \cdot (1 + e_{ss}) \cdot \left( \frac{\Theta_s}{\pi} \right)^{1/2} \) | (3.11)   |

| Solids pressure   | \( p_s = \alpha_s \cdot \rho_s \cdot \Theta_s + 2 \cdot \rho_s \cdot (1 + e_{ss}) \cdot \alpha_s^2 \cdot g_{\text{g,av}} \cdot \Theta_s \) | (3.12)   |

Radial distribution

| Arastoopour drag model | \( K_{gs} = \frac{17.3}{Re} + 0.336 \cdot \frac{\alpha_s \cdot \rho_g \cdot |\bar{\mathbf{v}}_s - \bar{\mathbf{v}}_g|}{d_s} \cdot \alpha_g^{-2.8} \) | (3.14)   |
|                       | \( Re = \frac{d_s \cdot \rho_g \cdot |\bar{\mathbf{v}}_s - \bar{\mathbf{v}}_g|}{\mu_g} \) | (3.15)   |

\( K_{gs} = \begin{cases} 
\frac{3}{4} \cdot C_D \cdot \frac{\alpha_s \cdot \alpha_g \cdot \rho_g \cdot |\bar{\mathbf{v}}_s - \bar{\mathbf{v}}_g|}{d_s} \cdot \alpha_g^{-2.65} & \text{for } \alpha_g > 0.8, \\
\frac{24}{\alpha_g \cdot Re_s} \left[ 1 + 0.15 \cdot (\alpha_g \cdot Re_s)^{0.687} \right] & \text{otherwise} 
\end{cases} \) (3.16)
Continued Table 3.2

For $\alpha_g \leq 0.8$,

$$K_{gs} = 150 \cdot \frac{\alpha_s^2 \cdot \mu_g}{\alpha_g \cdot d_s^3} + 1.75 \cdot \frac{\alpha_s \cdot \rho_g \cdot (\bar{v}_s - \bar{v}_g)}{d_s}$$  \hspace{1cm} (3.18)

Syamlal-O'Brien drag model

$$K_{gs} = \frac{3}{4} \cdot \frac{\alpha_s \cdot \alpha_g \cdot \rho_g}{\nu_{rs} \cdot d_s} \cdot C_D \cdot \left( \frac{Re_s}{\nu_{rs}} \right) \cdot (\bar{v}_s - \bar{v}_g)$$ \hspace{1cm} (3.19)

$$C_D = \left( 0.63 + \frac{4.8}{\sqrt{Re_s / \nu_{rs}}} \right)^2$$ \hspace{1cm} (3.20)

$$\nu_{rs} = 0.5 \cdot \left( A - 0.06 \cdot Re_s + \sqrt{(0.06 \cdot Re_s)^2 + 0.12 \cdot Re_s \cdot (2 \cdot B - A) + A^2} \right)$$ \hspace{1cm} (3.21)

With

$$A = \alpha_g^{4.14}$$ \hspace{1cm} (3.22)

and

$$B = P \cdot \alpha_g^{1.28} \text{ for } \alpha_g \leq 0.85$$ \hspace{1cm} (3.23)

$$B = \alpha_g^Q \text{ for } \alpha_g > 0.85$$ \hspace{1cm} (3.24)

where $P$ & $Q$ are specified based on minimum fluidization velocity [Appendix D].

<table>
<thead>
<tr>
<th>Gramular energy diffusion coefficient</th>
<th>$k_{gs} = \frac{150 \cdot \rho_s \cdot d_s \cdot \Theta_s}{384 \cdot (1 + \epsilon_{ss}) \cdot g_{0,ss} \cdot \left[ 1 + \frac{6}{5} \cdot \alpha_s \cdot g_{0,ss} \cdot (1 + \epsilon_{ss}) \right]^2}$ \hspace{1cm} (3.25)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Collision dissipation energy</td>
<td>$\gamma_{ss} = \frac{12 \cdot (1 - \epsilon_{ss}^2) \cdot g_{0,ss} \cdot \rho_s \cdot \alpha_s^2 \cdot \Theta_s^{3/2}}{d_s \cdot \sqrt{\pi}}$ \hspace{1cm} (3.26)</td>
</tr>
<tr>
<td>Transfer of kinetic energy</td>
<td>$\phi_{gs} = -3 \cdot K_{gs} \cdot \Theta_s$ \hspace{1cm} (3.27)</td>
</tr>
<tr>
<td><strong>Riser</strong></td>
<td>Inner diameter of the riser</td>
</tr>
<tr>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td><strong>H</strong></td>
<td>Height of the riser</td>
</tr>
<tr>
<td><strong>P</strong></td>
<td>Operating pressure</td>
</tr>
<tr>
<td><strong>T</strong></td>
<td>Operating temperature</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Gas</strong></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>U&lt;sub&gt;r&lt;/sub&gt;</strong></td>
<td>Superficial velocity</td>
<td>8 m/s</td>
</tr>
<tr>
<td><strong>μ&lt;sub&gt;G&lt;/sub&gt;</strong></td>
<td>Shear viscosity</td>
<td>$1.85 \times 10^{-5}$ kg/m s</td>
</tr>
<tr>
<td><strong>ρ&lt;sub&gt;G&lt;/sub&gt;</strong></td>
<td>Density</td>
<td>1.2 kg/m³</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Particles</strong></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>G&lt;sub&gt;s&lt;/sub&gt;</strong></td>
<td>Mass flux</td>
<td>453 kg/m²s</td>
</tr>
<tr>
<td><strong>ρ&lt;sub&gt;p&lt;/sub&gt;</strong></td>
<td>Particle density</td>
<td>1600 kg/m³</td>
</tr>
<tr>
<td><strong>d&lt;sub&gt;p&lt;/sub&gt;</strong></td>
<td>Particle average diameter</td>
<td>70 μm</td>
</tr>
<tr>
<td><strong>U&lt;sub&gt;mf&lt;/sub&gt;</strong></td>
<td>Particle minimum fluidization velocity</td>
<td>0.0032 m/s</td>
</tr>
<tr>
<td><strong>e</strong></td>
<td>Particle-particle coefficient of restitution</td>
<td>0.99</td>
</tr>
<tr>
<td><strong>e&lt;sub&gt;ω&lt;/sub&gt;</strong></td>
<td>Wall-particle coefficient of restitution</td>
<td>0.9, 0.95, 0.99</td>
</tr>
<tr>
<td><strong>φ</strong></td>
<td>Specularity coefficient</td>
<td>0, 0.5, 0.9</td>
</tr>
<tr>
<td><strong>α&lt;sub&gt;s,max&lt;/sub&gt;</strong></td>
<td>Maximum solid volume fraction</td>
<td>0.55</td>
</tr>
</tbody>
</table>
Fig. 3.1: Schematic diagram of CFB unit.

At Time=0
\( u_g = u_s = 0 \)
\( \alpha_e = 1 \)

Gas-Solid Outlet
\( P_{out} = 1 \text{ atm} \)
76 mm
6.1 m

Gas-Solid Inlet
Average \( U_a = 8 \text{ m/s} \)
\( \alpha_e = 0.55 \)
\( \Theta_e = 0.0005 \text{ m}^2/\text{s}^2 \)

Fig. 3.2: Schematic diagram of the 2-D riser with the boundary and initial conditions.
Fig. 3.3: Schematic of bottom part of the HDCF unit.
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Fig. 3.4: Solid volume fraction distribution (a), and (b) particle velocity distribution of the inlet section of the HDCFB riser.

Fig. 3.5: Radial profiles of solid volume fraction (a), and particle axial velocity (b) at riser inlet, \( Z = 0 \).
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Fig. 3.6: Radial profiles of solid volume fraction at Z = 3.8 m, (a) and axial profile of solid volume fraction (b) for different meshing densities.

Fig. 3.7: Radial Profiles of solid volume fraction (a) and axial particle velocity (b) for different specularity coefficient values, (Z = 3.8m, $e_w = 0.95$).
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Fig. 3.8: Radial profiles of solid volume fraction (a) and axial particle velocity (b) for different particle–wall restitution coefficient values, \( Z = 3.8 \) m.

Fig. 3.9: Radial profiles of solid volume fraction (a) and axial particle velocity (b) for different drag models, \( Z = 3.8 \) m, \( \phi = 0 \).
Fig. 3.10: Transient distributions of solid volume fraction in the middle section of the riser, $(Z = 3.2 \text{ m} - 4.4 \text{ m})$. 
Fig. 3.11: Transient distributions of axial particle velocity in the middle section of the riser, 
(Z = 3.2 m - 4.4 m).
Fig. 3.12: Comparison of laminar and turbulence models for radial (a) and axial (b) profiles of solid volume fraction, radial profiles of solid mass flux (c), and axial particle velocity (d); radial profiles were taken at $Z = 3.8$ m.
Fig. 3.13: Radial profiles of solid volume fraction (a) and axial particle velocity (b) predicted by simulation at $Z = 3.8$ m.
3.6 Literature Cited


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(20) Fluent Inc., Chapter 24.4: Eulrian Model, Fluent 6.2 Documentation, January, 2005, 26-44.


CHAPTER 4

4 CFD MODELING OF THE HYDRODYNAMICS OF A CIRCULATING FLUIDIZED BED UNDER VARIOUS FLUIDIZATION CONDITIONS: COMPARISON OF MODELING AND EXPERIMENTAL DATA

4.1 Introduction

Modeling circulating fluidized beds (CFB) hydrodynamics has become of interest over the past two decades because of their widespread industrial applications including cracking, drying, catalyst regeneration, power generation, and combustion [1]. The behavior of the gas/particle flow in CFB risers is particularly complex as the particles distribution in the riser gives a core-annular flow structure with dense clusters of particles flowing downward along the walls and dilute streams of particles moving upward in the center of the riser. The main objective of the models is to describe the complex hydrodynamics in order to assure valuable design and scale up of new units. The design process may lead to units being far from their optimal performance because of the sensitivity of the gas-particle flow to the scale and the operational condition [2].
With the development of high performance computers and advances in numerical techniques and algorithms, computational fluid dynamics (CFD) analysis of multiphase systems has grown over the past years and is anticipated to become a strong tool in the design and development of CFB units. Earlier simulation efforts focused on one dimensional models to compute gas-solid flows. Kunii and Levenspiel [3] and Li and Kwauk [4] provided models for predicting the axial behavior of solid density in the riser without considering radial distribution, which is characterized by the core-annular flow structure. More comprehensive models were then developed to predict the radial variation of the density of solids and the high average slipping velocities, accounting for two or more regions of different flow characteristics (e.g. core-annular flow) such as the one used by Pugsley [5], and Berruti et al. [6]. Recently, there has been a trend towards computing the gas-particle flow using three dimensional (3-D) models, with examples of authors applying these models being Petersen and Werther [7], Hua et al. [8], and Hansen et al. [9]. While recognizing that such complex systems are better studied in three dimensions to capture the detailed picture of the flow, with the current computational power two dimensional (2-D) models remain more popular. These 2-D models can provide valuable information for understanding the flow patterns with a reasonable computational effort.

Many authors, such as Benyahia et al. [10], Neri and Gidaspow [11], Chan et al. [12], and Zheng et al. [13], have achieved reasonable predictions of gas-solid hydrodynamics using the Eulerian-Eulerian model with the kinetic theory of granular flow. In the Eulerian-Eulerian approach, all the phases are modeled as interpenetrating continua with similar
conservation equations. The phases interact through additional source terms in the conservation equations. The kinetic theory of granular flow is based on the analogy between the thermal motion of the gas molecules in the kinetic theory of gases [14] and the random motion of solid particles. The development of the kinetic theory of granular solids started with the work of Chapman and Cowling [15]. Jenkins and Savage [16], Lun et al. [17], and Johnson and Jackson [18] continued the development of this theory. Sinclair and Jackson [19] first applied the kinetic theory of granular solid to model a multiphase flow in a pipe. Currently the kinetic theory of granular flow has become one of the most useful tools to model fluid-solid flows in dilute to dense bed regimes.

Although most of the industrial CFB reactors are operated with very high solid flux, which can reach up to \( \sim 1200 \text{ kg/m}^2\text{s} \) [20], the available models are mostly developed for more dilute systems with solid flux less than \( \sim 300 \text{ kg/m}^2\text{s} \). The high density circulating fluidized bed (HDCFB) operating with solid circulation rates above \( \sim 300 \text{ kg/m}^2\text{s} \) at a high superficial gas velocity \( \sim 6-10 \text{ m/s} \) characterized by Issangya et al. [21] is a new fluidization regime termed the dense suspension up-flow (DSU) regime. The DSU regime offers a more uniform radial solid distribution in comparison to the fast fluidization regime and unlike fast fluidization, there is no net solid down flow near the wall (i.e. no core-annular flow structure). To the author's knowledge, the most severe operating conditions that has been modeled so far were performed by S. Benyahia et al. [10], in which the solid circulation rate of 489 \( \text{ kg/m}^2\text{s} \) and the superficial gas velocity of up to 5.2 m/s was investigated. The flow under these conditions, however, showed downward
particle solid velocities near the wall, indicating that the fluidization had not reached the DSU regime.

Present research has modeled the riser section of a CFB using an Eulerian-Eulerian approach with kinetic theory of granular flow. While most of the CFD modeling works reported in the literature were evaluated for a single or over a limited operating conditions, the current model was evaluated against experimental findings of solid volume fraction, particle axial velocity, and solid mass flux for a wide range of operating conditions from low to high density circulating fluidized bed riser.

4.2 Experimental Description

The experimental date reported by Liu [22] on the hydrodynamics of CFB at various operating conditions was used for the evaluation of the CFD modeling results. The experimental apparatus consisted of a dual loop circulating fluidized bed with a multifunctional optical probe. This system involved a second riser of larger cross-sectional area (and therefore lower pressure drop) to lift the solids from the first riser to a higher level, facilitating a taller downcomer. The dual-loop circulating fluidized bed unit, shown schematically in Figure 4.1, consists of two Plexiglas vertical risers, two plexiglas downcomers, an impingement separator plate, three cyclones, two air root's blowers, and a bag house.

FCC particles of mean diameter 70μm and density 1600 kg/m³ were used. Experimental measurements were collected in the first riser of diameter 76 mm and height 6.1 m. A
dual functional-fiber optical probe was used to measure local particle volume fraction and local particle velocity simultaneously. This technique allows for estimating the local solid flux by integrating a multiplication of local particle volume fraction and local velocities over the riser cross section. Detailed description of the CFB system setup and the measuring technique can be reviewed at Liu et al. [22,23,24].

4.3 Modeling Description

An Eulerian-Eulerian model with the kinetic theory of granular flow was used to model the hydrodynamics of the gas-solid flow in the riser section of the CFB unit. One set of the mass and momentum conservation equations were solved for each phase, where the momentum equations were linked by an interphase exchange term. In the case of the isothermal condition without mass transfer, as considered in this study, the model governing equations for the gas and solid phase are as follows [25]:

4.3.1 Governing Equations

The continuity equation for each phase, $q$, is described by

$$\frac{\partial}{\partial t}(\alpha_q \cdot \rho_q) + \nabla \cdot (\alpha_q \cdot \rho_q \cdot \bar{v}_q) = 0$$

(4.1)

where $\alpha_q$, $\rho_q$, and $v_q$ are the volume fraction, density, and velocity of each phase, respectively.

The momentum equation for the gas phase, $g$, is given by

$$\frac{\partial}{\partial t} (\alpha_g \cdot \rho_g \cdot \bar{v}_g) + \nabla \cdot (\alpha_g \cdot \rho_g \cdot \bar{v}_g^2) =$$

$$-\alpha_g \cdot \nabla p + \nabla \cdot \bar{t}_g + \alpha_g \cdot \rho_g \cdot \bar{g} + K_{gs} \cdot (\bar{v}_g - \bar{v}_s)$$

(4.2)
and for the solid phase, \( s \), is given by
\[
\frac{\partial}{\partial t} \left( \alpha_s \cdot \rho_s \cdot \bar{v}_s \right) + \nabla \cdot \left( \alpha_s \cdot \rho_s \cdot \bar{v}_s^2 \right) = -\alpha_s \cdot \nabla p - \nabla p_s \\
+ \nabla \cdot \bar{\tau}_s + \alpha_s \cdot \rho_s \cdot \bar{g} + K_{ps} \cdot \left( \bar{v}_s - \bar{v}_g \right) + \sum_{i,j=1}^{N,M} \left( K_{sij} \cdot \left( \bar{v}_{si} - \bar{v}_{sj} \right) \right)
\]
(4.3)

where \( p, g, \bar{\tau}, \) and \( K \) are the fluid pressure, gravity, stress tensor and gas-solid drag coefficient, respectively.

The conservation equation for the fluctuation energy of solid phase, known as granular temperature, \( \Theta \), can be obtained by solving its transport equation, which has the form:
\[
\frac{3}{2} \left[ \frac{\partial}{\partial t} \left( \rho_s \cdot \alpha_s \cdot \Theta_s \right) + \nabla \cdot \left( \rho_s \cdot \alpha_s \cdot \bar{v}_s \cdot \Theta_s \right) \right] = \left( -p_s \bar{I} + \bar{p}_s \right) : \nabla \cdot \bar{v}_s \\
+ \nabla \cdot \left( k_{\Theta_s} \cdot \nabla \cdot \Theta_s \right) - \gamma_{\Theta_s} + \phi_{\Theta_s}
\]
(4.4)

where \( k_{\Theta_s} \) is the thermal diffusion coefficient, \( \gamma_{\Theta_s} \) is the collision dissipation energy, and \( \phi_{\Theta_s} \) is the transfer of kinetic energy between gas and solid phase. Definitions for these terms are given in Table 4.1.

### 4.3.2 Closure Laws

In order to solve the governing equations, several unknown terms required modeling. The models required for these unknown terms are known as closure laws. Appropriate closure laws are required for the corresponding stress tensors for each phase, solid phase pressure, and momentum interphase coefficient.

#### 4.3.2.1 Gas And Solid Phase Stress Tensor, \( \bar{\tau}_q \)

\( \bar{\tau}_q \) for each phase, \( q \), can be expressed as
\[
\tau_q = \alpha_q \cdot \mu_q \cdot \left( \nabla \cdot \vec{v}_q + \nabla \cdot \vec{v}_q^T \right) + \alpha_q \cdot \left( \lambda_q - \frac{2}{3} \cdot \mu_q \right) \cdot \nabla \cdot \vec{v}_q \bar{I} \tag{4.5}
\]

where \( \mu, \lambda, \bar{I} \) are shear and bulk viscosities and unit tensor, respectively. Definitions for these terms to close equation 4.5 are given in Table 4.1.

### 4.3.2.2 Solid Phase Pressure, \( P_s \)

The solid phase pressure is described in the context of the kinetic theory of granular flow as follows:

\[
P_s = \alpha_s \cdot \rho_s \cdot \Theta_s + 2 \cdot \rho_s \cdot (1 + e_{ss}) \cdot \alpha_s^2 \cdot g_{o,ss} \cdot \Theta_s \tag{4.6}
\]

where \( e_{ss} \) is particle-particle restitution coefficient, and \( g_{o,ss} \) is the radial distribution function. The radial distribution function can be interpreted as the probability of a single particle touching another particle in the solid phase. Thus, its value increases with increasing solid volume fraction. In this study, the following expression by Lun et al. [17] was used:

\[
g_{o,ss} = \left[ 1 - \left( \frac{\alpha_s}{\alpha_{s,\text{max}}} \right)^{1/3} \right]^{-1} \tag{4.7}
\]

### 4.3.2.3 Gas-Solid Interphase Exchange Coefficient, \( K_{gs} \)

For relatively small particles with density much larger than the continuous phase density, the interphase drag force dominates the other forces such as lift and virtual mass [26]. Therefore, the gas-solid momentum exchange coefficient, \( K_{gs} \), was assumed to have only the drag contribution. Since the gas-solid flow in the CFB riser possesses a non-uniform solid volume fraction distribution, a proper model to specify the gas-solid drag
coefficient for wide range (i.e. dilute to dense) of solid volume fraction should be used. There are several drag models applicable to the gas-solid flow in CFB risers in the literature, such as Gidaspow [27], Arastoopour [28], and Syamlal and O’Brien drag models [29]. As a result of the investigation, discussed earlier in Section 3.4.3, which involved applying different drag models for the same system modeled in this study, the Syamlal and O’Brien drag model with a modification for the actual particle minimum fluidization condition was found to result in a better modeling results compared to the Gidaspow and Arastoopour drag models. Therefore, this model was used in this study to model the gas-solid interphase exchange coefficient as follows:

\[ K_{gs} = \frac{3}{4} \cdot \frac{\rho_s}{\rho_g} \cdot \frac{d_s}{v_{r,s}} \cdot C_D \cdot \left( \frac{Re_s}{v_{r,s}} \right) \cdot |\bar{v}_s - \bar{v}_g| \]  

\[ C_D, \text{ the drag coefficient, is expressed as} \]
\[ C_D = \left( 0.63 + \frac{4.8}{\sqrt{Re_s/v_{r,s}}} \right)^2 \]

The solids Reynolds number, \( Re_s \), is calculated by
\[ Re_s = \frac{\rho_g \cdot d_s}{\mu_g} \cdot |\bar{v}_s - \bar{v}_g| \]
and \( v_{r,s} \), the terminal velocity is expressed by:
\[ v_{r,s} = 0.5 \cdot \left( A - 0.66 \cdot Re_s + \sqrt{(0.06 \cdot Re_s)^2 + 0.12 \cdot Re_s \cdot (2 \cdot B - A) + A^2} \right) \]

with
\[ A = \alpha_g^{4.14} \]
and
\[ B = P \cdot \alpha_g^{1.28} \text{ for } \alpha_g \leq 0.85 \]
\[ B = \alpha_g^Q \text{ for } \alpha_g > 0.85 \]

where \( P \) & \( Q \) are specified based on minimum fluidization velocity [Appendix D].
4.4 Solution Procedure

A commercial CFD package (Fluent Inc., V6.2) [25] was used to provide a numerical solution for the governing equations. The finite volume method by Patankar [30] was used to discretize the governing equations on computational grids. A second order upwind discretization schemes were used to solve the convection terms.

The calculations were performed using a 2-D computational domain with the dimensions of the domain in radial and axial direction being 0.075 m and 6.1 m, respectively; which are similar to those of the riser in which the experiments were performed. The computational domain consisted of 75 grids radially and 308 grids along the axis of the riser with a total of 21,560 grids resulting from this grid distribution. In the radial direction, the grid spacing was distributed non-uniformly; more cells were placed closer to the wall to capture the complex flow behavior in this region. Uniform grid spacing was used in the axial direction except at the outlet region where the grid spacing was decreased to better capture the exit effect. A schematic drawing of the mesh structure along with the initial and boundary conditions are shown in Figure 4.2.

According to Ferziger and Peric [31], in order to ensure the numerical accuracy and stability, the time step for modeling unsteady state conditions should be limited by a Courant number, C, which is a function of the smallest cell dimension, \( Z_{\text{min}} \), and the largest instantaneous velocity, \( u_{\text{max}} \), as follows:

\[
C = u_{\text{max}} \frac{\Delta t}{\Delta Z_{\text{min}}} \leq 1
\] (4.12)
CHAPTER 4: Comparison of Modeling and Experimental Data

Time steps of $5 \times 10^{-4} - 1 \times 10^{-3}$ s which correspond to the Courant numbers of 0.3-0.9 at various conditions were used, and the simulation was conducted for 45 s of real fluidization time, corresponding to 10-12 days of computational time on a 1.6 GHz workstation. In order to describe the complex hydrodynamics of gas-solid flow in CFB risers, flow variables should be averaged over a reasonable period of time after the quasi-steady-state conditions are reached for the outlet solid flux. Therefore, the time averaged distributions of flow variables were computed for the period of 17 to 45 s, which corresponds to the time after the solid mass flux at the riser outlet reached a quasi steady state condition. A convergence criterion of $1 \times 10^{-4}$ was specified for the relative error between two successive iterations.

The initial and boundary conditions used for the gas phase and particle phase applied in the simulation are given in Figure 4.2. At the inlet, all velocities and volume fractions of both phases were specified. A 2-D modeling of the J-valve at the inlet of the riser revealed that the inlet solid volume fraction and particles velocity are distributed non-uniformly at the inlet of the riser. Near the wall, the particles enter with their maximum packing limit at relatively low velocity, while in the central area, the particles volume fraction approaches zero. Based on this, the velocity profile provided in Figure 4.2 was used at the inlet and the inlet conditions ($u_s$ and $u_g$) were calculated for every case in this study to match the average superficial gas velocity and the total solid mass flux used in the experiments. More details of the inlet investigation were discussed earlier in Section (3.4.1). At the outlet, the pressure was specified (atmospheric). At the walls, the no-slip boundary condition can be specified for the gas phase. However, this condition will not
be realistic in the case of solid phase particles. The gas tangential and normal velocities and the normal velocity of the particles were set to zero. The following boundary equations applied for the solid tangential velocity and granular temperature at the wall:

\[
\begin{align*}
  u_{s,w} &= -\frac{6\alpha_s \mu_s}{\sqrt{3}\sqrt{\Theta \pi \rho_s \alpha_s g_{o,as}}} \frac{\partial u_{s,w}}{\partial n} \\
  \Theta_w &= -\frac{k\partial\Theta_w}{\gamma_w} + \frac{\sqrt{3}\pi \rho_s \alpha_s u_{s,\text{slip}} g_{o,as} \Theta^3/s}{6\alpha_{s,\text{max}} \gamma_w}
\end{align*}
\]  

(4.13)  

(4.14)

where \( \gamma_w \), is expressed in terms of wall restitution coefficient \( e_w \), as:

\[
\gamma_w = \frac{\sqrt{3}\pi(1-e_w^2)\alpha_s \rho_s g_{o,as} \Theta^{3/2}}{4\alpha_{s,\text{max}}}
\]  

(4.15)

These equations were developed by Johnson and Jackson [32]. As the authors expressed [35] the slip velocity between particles and the wall can be obtained by equating the tangential force exerted on the boundary and the particle shear stress close to the wall. Similarly, the granular temperature at the wall can be obtained by equating the granular temperature flux at the wall to the inelastic dissipation of energy, and to the generation of granular energy due to slip at the wall region. The flow parameters for the gas and solid used in the model are summarized in Table 4.2.

4.5 Results and Discussion

Several simulations have been performed with different modeling parameters and criteria in order to produce an adequate description of the two-phase flow behavior in the riser section of a high density circulating fluidized bed unit operating in a fast fluidization regime for specific operating condition (Case 1). The best comparisons between model
predictions and experimental data were obtained using the laminar viscous model, Syamlal and O'Brien drag model (modified based on the minimum fluidization velocity), and free-slip wall boundary condition (discussed earlier in Section 3.4.3). In order to investigate the limitations and capabilities of this model, the CFD model was evaluated for different operating conditions, ranging from the low to high density flow. The same modeling parameters were used for all the cases with varying only the superficial gas velocity, $U_g$, and/or solid mass flux, $G_s$, to match the experimental operating conditions. A summary of the various operating conditions of different cases are provided in Table 4.3.

### 4.5.1 High Density Riser (Fast Fluidization)

A comprehensive evaluation of the numerical model was performed by comparing model predictions and experimental results over various operating conditions within the same fluidization regime. Four case studies were performed with different solid mass fluxes, 455, 355, 325, and 254 kg/m$^2$s, and different superficial gas velocities 8, 6, 4, and 8 m/s, respectively.

Figures 4.3 and 4.4 capture a snapshot of the solid volume fraction and the axial particle velocity fields, respectively, for the middle section of the riser (3.4 m - 4.2 m) at 40 s simulation time from the beginning of the simulation. Combining these two figures, it is found that the flow along the riser has a core-annular flow structure which characterizes the fast fluidization regime. Dense solid phase accumulates and moves downward at the wall (the downward arrows in Figure 4.4), whereas a dilute solid phase moves upward in
the core of the riser. Cases 3 and 4 show clearly the formation of solid clusters (red colors in Figure 4.3) and the corresponding solid velocity and direction.

Figures 4.5 - 4.7 compare time averaged simulation predictions with experimental results for solid volume fraction, axial particle velocity, and solid mass flux, respectively. Time averaged hydrodynamic characteristics of the full cross section profiles is shown for Case 3 ($G_s = 325 \text{ kg/m}^2\text{s}$, and $U_g = 4 \text{ m/s}$) at $Z = 3.8 \text{ m}$. The flow information for the right half side of the riser at $Z = 3.8 \text{ m}$ is shown for Cases 1, 2, and 4 because there was no experimental data available over the full cross section area for these cases. Figures 4.5-4.7, case c showed that the model was capable of predicting the nearly axisymmetrical flow patterns for the case in which the full cross section profiles were measured, despite of the unsymmetrical configuration of the outlet geometry.

Figures 4.5 and 4.6 clearly illustrate the inherent core-annular flow structure of the solid phase for all the cases. The solids mainly accumulate and move downwards at the walls, whereas a dilute gas–particle stream flows upwards in the core of the riser with the maximum axial velocity. In general, the model predictions of solid volume fractions and axial particle velocities are in reasonable agreement with experimental results for all the cases. However, the solid volume fraction comparisons are less satisfactory near the wall. Most of the models available today are unable to describe this segregation well as reported in the previous studies (e.g. [10,11,33,34]) and therefore, underestimate the solids concentration at the walls. This discrepancy can be a result of some common simplifications that are assumed in the models to tolerate the computation limitations.
Identifying a mean value of solid particle sizes, which will behave in the same way as the population of the solid phase with specific particle size distribution, can result in a discrepancy in model predictions especially if the particle size distribution is not smooth and wide [26]. Mathisesen et al. [35] reported results of simulation with three solid phases, which show encouraging agreement with the experimental data. However, the computational requirements increase significantly with an increase in number of solid phases. In addition, accurate model predictions are difficult to obtain unless the real geometry was modeled in 3-D as opposed to 2-D.

Figure 4.7 shows a comparison of the predicted time averaged solids flux with experimental results. No direct measurement of the solid flux was performed experimentally, but its value was calculated by multiplying the instantaneous solid concentration and axial particle velocity, which were measured simultaneously using a dual functional optical probe, and then averaged for an extended time period. The same principle was applied in obtaining modeling values. The model agreed well with the experimental data qualitatively. The solid flux is at its maximum value near the center, while a downward flow of solids is predicted near the walls. However, the predictions are in greater agreement near the wall than the core area as the particle velocity is at its maximum in the central area and even small differences in the solid volume fraction can result in significant differences in the solid flux calculation in this region. Although cases 1-4 represent various operating conditions, their hydrodynamic profiles (Figures 4.5-4.7) display an overall similarity in pattern. It is evident that these cases are operating within the same fluidization regime and therefore have the same flow characteristics.
4.5.2 High Density Riser (Dense Suspension Up-flow, DSU)

Since the model has shown the capability of predicting the main characteristics of the complex gas-solid hydrodynamics in a HDCFB riser for high density fast fluidization regime (up to 455 Kg/m$^2$s), it was important to investigate its performance for a different fluidization regime at a higher solid mass flux. It was shown experimentally that at a solid mass flux of 550 kg/m$^2$s, the system has slightly more uniform radial solid distribution compared to the fast fluidization regime with no net solid downward flow near the wall (i.e. no core-annular flow pattern) [21]. Under these conditions, the flow is differentiated from the fast fluidization regime and is termed dense suspension up-flow (DSU). Figure 4.8 reveals the transient behavior of the axial particle velocity of a system operating at superficial gas velocity and solid mass flux of 8 m/s and 550 Kg/m$^2$s, respectively, for the middle section of the riser for the period from 8 to 45 s. The particles up-flow motion in the entire cross section of the bed is predicted by the model. However, this flow pattern does not maintain through the full height of the riser and around $Z = 3.8$ m, particles move downward along the walls. A comparison of the axial particle velocity distributions for the DSU (Case 5) with Cases 1 and 3 at different heights and $t = 40$ s is given in Figure 4.9. While the HDCFB riser operating in fast fluidization regimes countered near-wall particles downward flow for the entire section of the riser, the HDCFB riser operating in the DSU regime did not show particle downward flow for the lower section of the riser ($Z < 3.8$ m). This indicates that the model has predicted the DSU behavior in the lower section of the riser ($Z < 3.8$ m) and the fast fluidization behavior at the upper section ($Z > 3.8$ m). No experimental results were available for the upper section of the riser to evaluate this prediction.
The time averaged model predictions were compared to the experimental results in Figure 4.10. While the modeling results of the solid volume fraction partially agreed with the experimental results for the central area, they are significantly over-predicted near the wall (Figure 4.10a). The model predictions of the axial particle velocity match the experimental data at $r/R = 0.5$ to 0.9 (Figure 4.10b), but they were over predicted at the central area ($r/R = 0.0 - 0.5$). The downward particle velocities near the wall resulted in a downward solid flux (Figure 4.10c), whereas the experimental data showed no net downward flow of solid particles. It appears that the model did not predict the flow pattern of the DSU regime accurately. It is likely because of the implementation of inaccurate inlet conditions and possible sensitivity of DSU regime to the inlet conditions. Both feed geometry and flow conditions through the inlet cross section strongly affect the flow pattern in the riser. Predictions of relatively high solid volume fraction (comparing to experimental results) near the wall could have been contributed to the inaccurate predictions of solid flow near the wall at the upper part of the riser by the model.

4.5.3 Low Density Riser (Fast Fluidization)

CFB risers operating at relatively low solid fluxes (< 100 kg/m²s) and overall solid volume fractions less than about 10% are considered low density circulating fluidized beds [36]. A low density riser has also been considered in order to investigate the limitations and capabilities of this model for a wider range of operating conditions. CFD modeling predictions were compared to experimental results for solid mass flux and superficial gas velocity of 94 kg/m²s and 4 m/s, respectively. This model was capable of predicting the main feature of the gas-solid flow in CFB risers operating in fast...
fluidization regime which is the core-annular flow structure (Figure 4.11). However, a quantitative comparison between the time averaged predictions and experimental results for solid volume fraction and axial particle velocity, given in Figure 4.12, shows significant disagreement. The solid volume fraction predicted by the model, given in Figure 4.12a, were much higher at the center of the riser ($r/R = 0$) and much lower near the wall comparing to the experimental results. The axial particle velocity predictions, given in Figure 4.12b, showed relatively better agreement with experimental results but it was under predicted in the core area. The solid mass flux predictions, shown in Figure 4.12c, were significantly overestimated in the central area which resulted in lower predictions in the rest of the riser cross sectional area. Neri and Gidaspow [11] used the Eulerian-Granular model to describe the flow hydrodynamics of a low density riser with an overall solid volume fraction around 3-4%. Although the reported time averaged particle concentrations and fluxes showed the core annular flow regime and cluster formation, a comparison between simulation results and experimental data at the middle cross section of the riser showed significant dissimilarities. The core solid concentration profile was flatter with a remarkable difference as low as one third of that of the experimental data. Moreover, the axial particle velocity at the center was twice higher than that of the experimental data. On the other hand, Chan et al. [12] and Zheng et al. [13] reported satisfactory agreements of modeling results with experimental data for low density risers with turbulence modulation. The $k-\varepsilon-k_p-\varepsilon_p$ resulted in more reasonable axial particle velocity distribution in the core area and solid volume fraction distribution in the annulus region, when compared with the $k-\varepsilon$ turbulence models where only the turbulence of gas phase is considered and the $k-\varepsilon-k_p$ where the
dissipation of particles kinetic energy is not considered. This might be an indication of the importance of the turbulence factors, in particular the solid phase turbulence in gas-solid flow behaviour when modeling low density risers.

4.6 Conclusion

A 2-D Eulerian-Eulerian model incorporating the kinetic theory of granular flow was developed to describe the hydrodynamics of gas-solid flow in the riser section of a HDCFB. A comprehensive numerical model evaluation by comparing experimental results from the literature was investigated for various operating conditions. It was found that a single model is capable of predicting the main features of the complex gas-solids flow for different operating condition within the high density fast fluidization regime satisfactorily. The predicted solid volume fraction and axial particle velocity were reasonably in good agreement with the experimental data. The developed model was capable of predicting the core-annular flow pattern and the cluster formation of the solid phase. However, the model was incapable of accurately predicting the gas-solid flow behavior in low density circulating fluidized bed riser and risers operating in a dense suspension up-flow regime. Hence, the present model should be improved to obtain better predictions at different fluidization regimes.
Table 4.1: Constitutive equations

\[
k_{\Theta_s} = \frac{150 \cdot \rho_s \cdot d_s \sqrt{\Theta_s \cdot \pi}}{384 \cdot (1 + e_{ss}) \cdot g_{0,ss}} \left[ 1 + \frac{6}{5} \cdot \alpha_s \cdot g_{0,ss} \cdot (1 + e_{ss}) \right]^2 + \tag{4.16}
\]

\[
2 \cdot \rho_s \cdot d_s \cdot \alpha_s^2 \cdot g_{0,ss} \cdot (1 + e_{ss}) \cdot \sqrt{\Theta_s \cdot \pi} \tag{4.17}
\]

\[
\gamma_{\Theta ss} = \frac{12 \cdot \left( 1 - e_{ss}^2 \right) \cdot g_{0,ss} \cdot \rho_s \cdot \alpha_s^2 \cdot \Theta_s^{3/2}}{d_s \cdot \sqrt{\pi}} \tag{4.18}
\]

\[
\phi_{gs} = -3 \cdot K_{gs} \cdot \Theta_s \tag{4.19}
\]

\[
\mu_s = \mu_{s,\text{col}} + \mu_{s,\text{kin}} + \mu_{s,\text{fr}} \tag{4.20}
\]

\[
\mu_{s,\text{col}} = \frac{4}{5} \cdot \alpha_s \cdot \rho_s \cdot d_s \cdot g_{0,ss} \cdot (1 + e_{ss}) \cdot \left( \frac{\Theta_s}{\pi} \right)^{1/2} \tag{4.21}
\]

\[
\mu_{s,\text{kin}} = \frac{10 \cdot \rho_s \cdot d_s \cdot \sqrt{\Theta_s \cdot \pi}}{96 \cdot \alpha_s \cdot (1 + e_{ss}) \cdot g_{0,ss}} \left[ 1 + \frac{4}{5} \cdot g_{0,ss} \cdot \alpha_s \cdot (1 + e_{ss}) \right]^2 \tag{4.22}
\]

\[
\mu_{s,\text{fr}} = \frac{p_s \cdot \sin \phi}{2 \cdot \sqrt{I_{2D}}} \tag{4.23}
\]

\[
\lambda_s = \frac{4}{3} \cdot \alpha_s \cdot \rho_s \cdot d_s \cdot g_{0,ss} \cdot (1 + e_{ss}) \cdot \left( \frac{\Theta_s}{\pi} \right)^{1/2} \tag{4.24}
\]
### Table 4.2 Flow parameters used in the numerical models

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gas density, $\rho_g$</td>
<td>1.2 kg/m$^3$</td>
</tr>
<tr>
<td>Gas viscosity, $\mu_g$</td>
<td>$1.85 \times 10^{-5}$ kg/ms</td>
</tr>
<tr>
<td>Solid density, $\rho_p$</td>
<td>1600 kg/m$^3$</td>
</tr>
<tr>
<td>Particle average diameter, $d_p$</td>
<td>70 μm</td>
</tr>
<tr>
<td>Particle minimum fluidization velocity, $U_{mf}$</td>
<td>0.0032 m/s</td>
</tr>
<tr>
<td>Particle-particle coefficient of restitution, $e$</td>
<td>0.99</td>
</tr>
<tr>
<td>Maximum solid volume fraction, $\alpha_{s,max}$</td>
<td>0.55</td>
</tr>
</tbody>
</table>

### Table 4.3: Summary of operating conditions with corresponding numeric values

<table>
<thead>
<tr>
<th>Operating Condition</th>
<th>High Density (Fast Fluidization)</th>
<th>High Density (DSU)</th>
<th>Low Density (Fast Fluidization)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Case 1</td>
<td>Case 2</td>
<td>Case 3</td>
</tr>
<tr>
<td>$G_s$ (kg/m$^2$ s)</td>
<td>455</td>
<td>355</td>
<td>325</td>
</tr>
<tr>
<td>$U_g$ (m/s)</td>
<td>8</td>
<td>6</td>
<td>4</td>
</tr>
</tbody>
</table>
Fig. 4.1: Schematic diagram of CFB unit

Outlet

\[ P = 1 \text{ atm.} \]

0.076 m

\[ \frac{4}{14} \]

At \( t = 0 \)

\[ u_s = 0 \]

\[ u_q = 0 \]

\[ \xi_g = 1 \]

Wall

\[ \phi = 0, \epsilon_w = 0.95, \]

\[ u_{g,wall} = v_{g,wall} = v_{s,wall} = 0 \]

\[ u_{s,wall} \neq 0 \]

Inlet

0.1 m

\[ 15 \text{ mm} \]

\[ 46 \text{ mm} \]

\[ 15 \text{ mm} \]

\[ \square \text{ Gas, } \xi_g = 1, u_{s,\text{in}} = 0, u_{g,\text{in}} \]

\[ \square \text{ Gas/Solid, } \xi_g = 0.45, u_{g,\text{in}} \& u_{s,\text{in}} \]

Fig. 4.2: Schematic diagram of the 2-D riser with inlet, outlet, and initial conditions.
Fig. 4.3: Transient Distributions of solid volume fraction at the middle section of the riser, $Z = 3.4 - 4.2$ m, at $t = 40$ s; (Case 1: $U_g = 8$ m/s, $G_r = 455$ kg/m$^2$s, Case 2: $U_g = 6$ m/s, $G_r = 355$ kg/m$^2$s, Case 3: $U_g = 4$ m/s, $G_r = 325$ kg/m$^2$s, Case 4: $U_g = 8$ m/s, $G_r = 254$ kg/m$^2$s).

Fig. 4.4: Distributions of axial particle velocity in the middle section of the riser, $Z = 3.4 - 4.2$ m, at $t = 40$ s (Case 1: $U_g = 8$ m/s, $G_r = 455$ kg/m$^2$s, Case 2: $U_g = 6$ m/s, $G_r = 355$ kg/m$^2$s, Case 3: $U_g = 4$ m/s, $G_r = 325$ kg/m$^2$s, Case 4: $U_g = 8$ m/s, $G_r = 254$ kg/m$^2$s).
Fig. 4.5: Radial profiles of time averaged solid volume fraction at Z = 3.8 m (Case 1: \( U_g = 8 \) m/s, \( G_s = 455 \) kg/m²s, Case 2: \( U_g = 6 \) m/s, \( G_s = 355 \) kg/m²s, Case 3: \( U_g = 4 \) m/s, \( G_s = 325 \) kg/m²s, Case 4: \( U_g = 8 \) m/s, \( G_s = 254 \) kg/m²s).
Fig. 4.6: Radial profiles of time-averaged axial particle velocity at Z = 3.8 (Case 1: $U_g = 8$ m/s, $G_v = 455$ kg/m$^2$s, Case 2: $U_g = 6$ m/s, $G_v = 355$ kg/m$^2$s, Case 3: $U_g = 4$ m/s, $G_v = 325$ kg/m$^2$s, Case 4: $U_g = 8$ m/s, $G_v = 254$ kg/m$^2$s).
Fig. 4.7: Radial profile of time averaged solid mass flux at $Z = 3.8$ m (Case 1: $U_g = 8$ m/s, $G_s = 455$ kg/m$^2$s, Case 2: $U_g = 6$ m/s, $G_s = 355$ kg/m$^2$s, Case 3: $U_g = 4$ m/s, $G_s = 325$ kg/m$^2$s, Case 4: $U_g = 8$ m/s, $G_s = 254$ kg/m$^2$s).
Fig. 4.8: Transient Distributions of axial particle velocity in the middle section of the riser, Z= 3.4 - 4.2 m,
(Case 5: $U_g = 8 \text{ m/s}, G_s = 550 \text{ kg/m}^2\text{s}$).
Fig. 4.9: Distributions of axial particle velocity at different heights, at \( t = 40 \) s (Case 1: \( U_g = 8 \) m/s, \( G_s = 455 \) kg/m\(^2\)s, Case 3: \( U_g = 4 \) m/s, \( G_s = 325 \) kg/m\(^2\)s, Case 5: \( U_g = 8 \) m/s, \( G_s = 550 \) kg/m\(^2\)s).
Fig. 4.10: Radial profiles of time averaged solid volume fraction at Z = 3.8 m (a), axial particle velocity (b), and solid mass flux (c) (Case 5: \( U_g = 8 \) m/s, \( G_s = 550 \) kg/m\(^2\)s).
Fig. 4.11: Transient Distributions of solid volume fraction (on top) and axial particle velocity (bottom) for the middle section, \( Z = 3.4 - 4.2 \text{ m} \), of the riser (Case 6: \( U_g = 4 \text{ m/s} \), \( G_r = 94 \text{ kg/m}^2\text{s} \)).
Fig. 4.12: Radial profiles of time averaged solid volume fraction at $Z = 3.8$ m (a), axial particle velocity (b), and solid mass flux (c) (Case 6: $U_g = 4$ m/s, $G_s = 94$ kg/m$^2$s).
4.7 Literature Cited


(22) Liu, J., Particle and gas dynamics of high density circulating fluidized beds, PHD Thesis 2001, The University of British Columbia, Vancouver, BC.

(23) Liu, J., Grace, J., and Bi, H., Radial distribution of local particle velocity in a high density circulating fluidized bed riser, 7th Circulating fluidized bed, CSChE national conference 2002, Ottawa.


CHAPTER 5: Conclusions and Recommendations

CHAPTER 5

5 Conclusions and Recommendations

This thesis presents the two dimensional multiphase modeling of gas-solid flow in the riser section of a circulating fluidized bed. Model predictions have been evaluated against experimental data from the literature. Conclusions of this work and recommendations for future work are given in the following sections.

5.1 Conclusions

A 2-D Eulerian-Eulerian model incorporating the kinetic theory of granular flow was developed using Fluent V6.2 to describe the hydrodynamics of gas-solid flow in the riser section of a HDCFB. Several simulations have been performed in order to investigate the effect of different operating conditions, model parameters, and to generate an adequate description of the observed two-phase flow patterns in the riser of the CFB. The model was able to predict most of the gas-solid flow characteristics in a circulating fluidized bed riser. The core-annular flow structure which characterizes CFB risers operating in fast fluidization regimes was observed by this model. The model also predicted the solid down-flow in the form of clusters near the walls with the predictions being nearly
CHAPTER 5: Conclusions and Recommendations

symmetric with respect to the riser axis despite of the unsymmetrical configuration of the outlet geometry.

A parametric study was performed in order to examine several modeling parameters, including the restitution coefficient, specularity coefficient, and interphase drag coefficients. Using free-slip boundary condition (equivalent to specularity coefficient equal to zero, $\phi = 0$), the CFD model predictions of the solid volume fraction near the wall agreed better with the experimental data, while the implementation of no-slip and relatively high slip boundary condition significantly underestimated the solid volume fraction near the wall. Varying the wall restitution coefficient values did not affect model predictions for the solid volume fraction or for axial particle velocity. Calculating the gas–solid momentum interphase exchange coefficient using the Gidaspow, Arastoopour, and Syamlal and O'Brien drag models was found to result in similar predictions of the solid volume fraction and axial particle velocity profiles. However, the Syamlal and O'Brien drag model resulted in a better solid concentration prediction at the core area.

A comprehensive numerical model evaluation against experimental results from the literature was investigated for a broad range of operating conditions including the low to high density risers. It was found that within the high density fast fluidization regime, model predictions are qualitatively in good agreement with experimental results for different operating conditions. However, the model was incapable of accurately predicting the gas-solid flow behavior in low density circulating fluidized bed riser and...
risers operating at a dense suspension up-flow regime. Hence, the present model should be improved to obtain better predictions at different fluidization conditions.

5.2 Recommendations

The recommendations for future work are as follows:

- Due to the current computational limitations, a two dimensional representation of the system was modeled with the particles considered mono-dispersed. Once sufficient computational recourses are available, a three dimensional gas-solid flow simulation along with consideration of particle size distribution may render more realistic predictions.

- The model was verified against a broad range of operating condition for one specific system. More experimental data from the literature should be used for different CFB risers of various dimension and operating conditions to further demonstrate the model capabilities and limitations.

- The turbulence model applied in this work assumes the primary phase has the dominant role in the overall system turbulence. The model calculates the turbulence fluctuations of the secondary phase as a function of primary phase. A more general multiphase turbulence model is recommended to be used by solving one set of $k$ and $\varepsilon$ transport equations for each phase.

- This model studied the particle behavior in the riser and feeding system separately without considering the effect of both sections on one another especially at the inlet section of the riser. In order to produce a more realistic case, a combined geometry should be considered in one model.
APPENDICIES

Appendix A: Meshing
Appendix B: Drag Models
Appendix C: Data Extraction (Schemes and Macros)
Appendix D: Inlet Investigation
Appendix E: Turbulence Model
Appendix A: Meshing

GAMBIT 2.2.30 from Fluent Inc. was used to create 2-D geometry and structured meshes for Fluent. Schematic drawings of different mesh density for the bottom section, the top section, and the inlet section (J valve) are shown in this appendix.
The Entire System

Fig. A.1: Schematic diagram of the entire system.
APPENDIX

The Middle Section

Fig. A.2: Mesh density for (a) 10k grids (50 x 200),
(b) 21k grids (75 x 308), (c), 40k (100 x 400) (radial x vertical).
APPENDIX

The Top Section

Fig. A.3: Meshing and outlet Geometry of outlet section for 21k grids.
APPENDIX

The inlet Section (J-valve)

Fig. A.4: Meshing and outlet Geometry of inlet section (14k grids).
Appendix B: Drag Models

The procedure applied to specify the parameters $P$ and $Q$ for the corresponding minimum fluidization velocity in the Syamlal and O'Brien drag model (equations 3.21 and 4.11) is explained in this appendix. User defined functions (UDFs) of Fluent software allow a user to customize FLUENT to fit his particular modeling needs in order to enhance the existing FLUENT models. UDF used to modify the original Syamlal and O'Brien drag model and to define an additional drag model, Arastoopour, is provided.
APPENDIX

**Procedure for Specifying P and Q Values**

In order to modify the original Syamlal and O'Brien drag model for the minimum fluidization velocity, the corresponding values of the parameters $P$ and $Q$ have to be specified. The value of $B$ in equation B.5 should be varied by altering the value of $P$ (initial value, $P = 0.8$) until the $v_g$ calculated by equation B.1 equal the minimum fluidization velocity provided experimentally. The value of $Q$ (initial value, $Q = 2.65$) is then corrected by equation (D.6). Finally, the gas-solid exchange coefficient can be modeled by using the new values of $P$ and $Q$.

\[ v_g = \frac{\alpha_g \mu_g}{\rho_g d_p} \]  \hspace{1cm} (B.1)

$Re_t$, the Reynolds number under terminal settling conditions for the multiparticle system, is given by

\[ Re_t = v_{rs} Re_{tr} \]  \hspace{1cm} (B.2)

$Re_{tr}$, the Reynolds number under terminal settling conditions for a single particle, is given by Syamlal and O'Brien (1987) as follows

\[ Re_{tr} = \left( \frac{\sqrt{4.8^2 + 2.52\sqrt{4Ar/3} - 4.8}}{1.26} \right)^2 \]  \hspace{1cm} (B.3)

$Ar$, Archimedes number, is expressed as

\[ Ar = \frac{(\rho_s - \rho_g) d_p^3 \rho_g g}{\mu_g} \]  \hspace{1cm} (B.4)

By combining Equations 4.11 and B.2 one arrives at

\[ v_{rs} = \frac{A + 0.06BRe_{tr}}{1 + 0.06Re_{tr}} \]  \hspace{1cm} (B.5)

The following equation can be used to correct the value of $Q$:
$$Q = 1.28 + \log(P) / \log(0.85)$$  \hspace{1cm} (B.6)
UDF for modified Syamlal and O'Brien drag model

#include "udf.h"
#include "sg_mphase.h"

#define pi 4.*atan(1.)
#define diamsol 70e-6

DEFINE_EXCHANGE_PROPERTY(custom_drag_syalmlal, cell, mix_thread, s_col, f_col)
{
  Thread *thread_gas, *thread_sol;
  real x_vel_g, x_vel_s, y_vel_g, y_vel_s, abs_v, slip_x, slip_y,
       rho_g, rho_s, mu_g, rey_sol, afac, CD,
       bfac, void_g, v_term, f_drag, tau_sol, k_g_s;

  /* find the threads for the gas (primary) and solids (secondary phases).
   These phases appear in columns 2 and 1 in the Interphase panel respectively */

  thread_gas = THREAD_SUB_THREAD(mix_thread, s_col); /* gas phase */
  thread_sol = THREAD_SUB_THREAD(mix_thread, f_col); /* solid phase */

  /* find phase velocities and properties */
  x_vel_g = C_U(cell, thread_gas);
  y_vel_g = C_V(cell, thread_gas);
  x_vel_s = C_U(cell, thread_sol);
  y_vel_s = C_V(cell, thread_sol);

  slip_x = x_vel_g - x_vel_s;
  slip_y = y_vel_g - y_vel_s;

  rho_g = C_R(cell, thread_gas);
  rho_s = C_R(cell, thread_sol);

  mu_g = C_MU_L(cell, thread_gas); /* laminar viscosity */

  /* slip */
  abs_v = sqrt(slip_x*slip_x + slip_y*slip_y);

  /* solids reynolds number */
  rey_sol = rho_g*abs_v*diamsol/mu_g;

  /* particulate relaxation time */
APPENDIX

tau_sol = rho_s*diam_sol*diam_sol/(18.*mu_g);

/* gas vol frac*/
void_g = C_VOF(cell, thread_gas);

/* coefficients for terminal velocity correlation for the solid phase*/
afac = pow(void_g, 4.14);

if(void_g<=0.85)
    bfac = 0.1214*pow(void_g, 1.28);
else
    bfac = pow(void_g, 14.25488);

/* terminal velocity correlation for the solid phase */
v_term = 0.5*(afac-0.06*rey_sol+sqrt(0.0036*rey_sol*rey_sol+0.12*rey_sol*(2.*bfac-
afac)+afac*afac));

/* drag coefficient */
CD=pow((0.63+4.8/(sqrt(rey_sol/v_term))),2);

/* drag function */
f_drag = CD*rey_sol*void_g/(24*v_term);

/* fluid-solid exchange coefficient */
k_g_s = (1.-void_g)*rho_s*f_drag/tau_sol;

return k_g_s;
}
APPENDIX

UDF for Arastoopour drag model

#include "udf.h"
#include "sg_mphase.h"

#define pi  4.*atan(1.)
#define diamsol 70e-6

DEFINE_EXCHANGE_PROPERTY(arastoopour_drag_law, cell, mix_thread, s_col, f_col)
{
    Thread *thread_gas, *thread_sol;
    real x_vel_g, x_vel_s, y_vel_g, y_vel_s, abs_v, slip_x, slip_y,
        rho_g, rho_s, mu_g, rey_sol, void_g, k_g_s;

    /* find the threads for the gas (primary) and solids (secondary phases). */
    /* These phases appear in columns 2 and 1 in the Interphase panel respectively */
    thread_gas = THREAD_SUB_THREAD(mix_thread, s_col); /* gas phase */
    thread_sol = THREAD_SUB_THREAD(mix_thread, f_col); /* solid phase */

    /* find phase velocities and properties */
    x_vel_g = C_U(cell, thread_gas);
    y_vel_g = C_V(cell, thread_gas);
    x_vel_s = C_U(cell, thread_sol);
    y_vel_s = C_V(cell, thread_sol);

    slip_x = x_vel_g - x_vel_s;
    slip_y = y_vel_g - y_vel_s;

    rho_g = C_R(cell, thread_gas);
    rho_s = C_R(cell, thread_sol);

    mu_g = C_MU_L(cell, thread_gas); /* laminar viscosity */

    /* slip */
    abs_v = sqrt(slip_x*slip_x + slip_y*slip_y);

    /* solids reynolds number */
    rey_sol = rho_g*abs_v*diam_sol/mu_g;

    /* gas vol frac */
    void_g = C_VOF(cell, thread_gas);
/* fluid-solid exchange coefficient */

```c
k_g_s = (17.3/rey_sol+0.3336)*rho_g/diam_sol*abs_v*(1-void_g)/pow(void_g,2.8);

return k_g_s;
```

APPENDIX
Appendix C: Data Extraction: Schemes and Macros

Fluent contains two interface methods. Graphic User Interface (GUI) and Text User Interface (TUI). The (TUI) is written in a text form called Scheme. Schemes allow users to create a sequence of Fluent commands such as reading, writing and plotting data. In the present work schemes were used to generate data and then save them as data files for use in other program (Excel). Macros were then used to export data to Excel for post-processing and visualization. This section has examples of some schemes and macros that have been used in this work.
Scheme to Extract Data From Fluent

Title: Data Extraction Scheme
Purpose: This scheme extracts Particle volume fraction and axial velocity profiles from Fluent

(ti-menu-load-string "file/read-data HDCFB_vg8_Gs455_10000.dat")
(ti-menu-load-string "plot/plot yes vof 10 no no no solid vof yes 0 h.7 h1.4 h2.1 h2.8 h3.5 h4.2 h4.9 h5.6 h6.3 ( )")
(ti-menu-load-string "plot/plot yes vel 10 no no no solid v-velocity yes 0 h.7 h1.4 h2.1 h2.8 h3.5 h4.2 h4.9 h5.6 h6.3 ( )")
(ti-menu-load-string "file/read-data HDCFB_vg8_Gs455_10100.dat")
(ti-menu-load-string "plot/plot yes vof 10.1 no no no solid vof yes 0 h.7 h1.4 h2.1 h2.8 h3.5 h4.2 h4.9 h5.6 h6.3 ( )")
(ti-menu-load-string "plot/plot yes vel 10.1 no no no solid y-velocity yes 0 h.7 h1.4 h2.1 h2.8 h3.5 h4.2 h4.9 h5.6 h6.3 ( )")
(ti-menu-load-string "file/read-data HDCFB_vg8_Gs455_10200.dat")
(ti-menu-load-string "plot/plot yes vof 0.2 no no no solid vof yes 0 h.7 h1.4 h2.1 h2.8 h3.5 h4.2 h4.9 h5.6 h6.3 ( )")
(ti-menu-load-string "plot/plot yes vel 0.2 no no no solid y-velocity yes 0 h.7 h1.4 h2.1 h2.8 h3.5 h4.2 h4.9 h5.6 h6.3 ( )")
(ti-menu-load-string "file/read-data HDCFB_vg8_Gs455_10300.dat")
(ti-menu-load-string "plot/plot yes vof 0.3 no no no solid vof yes 0 h.7 h1.4 h2.1 h2.8 h3.5 h4.2 h4.9 h5.6 h6.3 ( )")
(ti-menu-load-string "plot/plot yes vel 0.3 no no no solid y-velocity yes 0 h.7 h1.4 h2.1 h2.8 h3.5 h4.2 h4.9 h5.6 h6.3 ( )")
(ti-menu-load-string "file/read-data HDCFB_vg8_Gs455_10400.dat")
(ti-menu-load-string "plot/plot yes vof 0.4 no no no solid vof yes 0 h.7 h1.4 h2.1 h2.8 h3.5 h4.2 h4.9 h5.6 h6.3 ( )")
(ti-menu-load-string "plot/plot yes vel 0.4 no no no solid y-velocity yes 0 h.7 h1.4 h2.1 h2.8 h3.5 h4.2 h4.9 h5.6 h6.3 ( )")
(ti-menu-load-string "file/read-data HDCFB_vg8_Gs455_10500.dat")
(ti-menu-load-string "plot/plot yes vof 0.5 no no no solid vof yes 0 h.7 h1.4 h2.1 h2.8 h3.5 h4.2 h4.9 h5.6 h6.3 ( )")
(ti-menu-load-string "plot/plot yes vel 0.5 no no no solid y-velocity yes 0 h.7 h1.4 h2.1 h2.8 h3.5 h4.2 h4.9 h5.6 h6.3 ( )")
(ti-menu-load-string "file/read-data HDCFB_vg8_Gs455_10600.dat")
(ti-menu-load-string "plot/plot yes vof 0.6 no no no solid vof yes 0 h.7 h1.4 h2.1 h2.8 h3.5 h4.2 h4.9 h5.6 h6.3 ( )")
(ti-menu-load-string "plot/plot yes vel 0.6 no no no solid y-velocity yes 0 h.7 h1.4 h2.1 h2.8 h3.5 h4.2 h4.9 h5.6 h6.3 ( )")
(ti-menu-load-string "file/read-data HDCFB_vg8_Gs455_10700.dat")
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(ti-menu-load-string "plot/plot yes vof 0.7 no no no solid vof yes 1 0 h 1.7 h 1.4 h 2.1 h 2.8 h 3.5 h 4.2 h 4.9 h 5.6 h 6.3 ( )")
Macro for Importing Data to Excel

Sub Volume_fraction_data_extraction()

' Volume_fraction_data_extraction Macro
' Macro recorded 2005/10/12 by Adnan

With ActiveSheet.QueryTables.Add(Connection:= "TEXT;E:\Adnan\Theses\HDCFB\gidaspow\vof38.9", Destination:=Range("BG1"))
.Name = "vof38.9"
.FieldNames = True
.RowNumbers = False
.FillAdjacentFormulas = False
.PreserveFormatting = True
.RefreshOnFileOpen = False
.RefreshStyle = xlInsertDeleteCells
.SavePassword = False
.SaveData = True
.AdjustColumnWidth = True
.RefreshPeriod = 0
.TextFilePromptOnRefresh = False
.TextFilePlatform = 437
.TextFileStartRow = 1
.TextFileParseType = xlDelimited
.TextFileTextQualifier = xlTextQualifierDoubleQuote
.TextFileConsecutiveDelimiter = False
.TextFileTabDelimiter = True
.TextFileSemicolonDelimiter = False
.TextFileCommaDelimiter = False
.TextFileSpaceDelimiter = False
.TextFileColumnDataTypes = Array(1, 1)
.TextFileTrailingMinusNumbers = True
.Refresh BackgroundQuery:=False
End With

With ActiveSheet.QueryTables.Add(Connection:= "TEXT;E:\Adnan\Theses\HDCFB\gidaspow\vof39", Destination:=Range("BI1"))
.Name = "vof39"
.FieldNames = True
.RowNumbers = False
.FillAdjacentFormulas = False
.PreserveFormatting = True
Appendix D: Inlet Investigation
Inlet Investigation

In the present work, an accurate modeling of the inlet conditions was impossible, because there were no observations or measurements provided for the inlet conditions during the experiments. Miller and Gidaspow (1992) reported that an exact inlet condition is difficult to measure due to its transient nature and as a consequence their accuracy is usually low. Therefore, different inlet conditions (uniform and non-uniform) were modeled in order to investigate the sensitivity of the simulation predictions to the inlet condition. The uniform inlet condition has the same values of the inlet solid volume fraction, \( \alpha_s \), the inlet solid velocity, \( u_s \), and the inlet gas velocity, \( u_g \), over the inlet cross sectional area, which correspond to the experimental operating condition of solid mass flux, \( G_s \), and superficial gas velocity, \( U_g \). The non-uniform inlet condition, which has different values of the inlet parameters, was defined numerically as follows:

The inlet section was examined initially by modeling the J-valve solely without considering the riser (Figure D.1). It was found that the riser inlet has non-uniform particles volume fraction and axial particle velocity distributions (Figure D.2). The particles were dragged vertically toward the wall without interfering in the gas flow. However, in order to generate a more realistic modeling a combined geometry of the inlet section and the riser was modeled (Figure D.3). Figure D.4 shows the radial profile of particles volume fraction and particles axial velocity at the riser inlet. The particles entered the riser at their maximum packing limit of 0.55 with velocity as low as 2 m/s near the right wall, while the particle volume fraction approaching zero in the rest of the inlet cross section. In order to model an entrance zone in 2-D geometry with entrance
velocity profile similar to that of 3-D system, the non-uniform inlet condition was defined by using velocity profiles similar to those given in figure D.4 near the two walls of the 2-D (Figure D.5). Figure D.6 compares model predictions using the uniform and non-uniform inlet conditions with experimental results. While the non-uniform inlet distribution model correctly predicted the flow hydrodynamics, the uniform inlet distribution model failed to predict most of the gas-solid flow behaviors. The overall solid volume fraction was underestimated significantly (Figure D.6a and b) when one compares the experimental and the non-uniform inlet distribution model. The particle velocity was also lower than the core particle velocity (Figure D.6d). This comparison shows that the implementation of correct inlet conditions is critical for the successful simulation of the flow hydrodynamics.
Fig. D.1: Solid volume fraction distribution (a), and particle velocity distribution (b) of the inlet section of the HDCFB riser, (J-valve model).

Fig. D.2: Radial profiles of solid volume fraction (a), and particle axial velocity (b) at riser inlet, (Z = 0, J-valve model).
APPENDIX

Fig. D.3: Solid volume fraction distribution (a), and particle velocity distribution (b) of the inlet section of the HDCFB riser, (J-valve + riser model).

Fig. D.4: Radial profiles of solid volume fraction (a), and particle axial velocity (b) at riser inlet, (Z = 0, J-valve + riser model).
Inlet

15mm 46mm 15mm

Outlet

Gas, $\alpha_g = 1$, $u_{s,in} = 0$, $u_g = 13$ m/s
Gas/Solid, $\alpha_g = 0.45$, $u_{g,in} = u_s = 1.3$ m/s

Fig. D.5: Schematic diagram of the 2-D riser with non-uniform inlet condition.
Fig. D.6: Radial (a) and axial (b) profiles of solid volume fraction, radial profiles of solid mass flux (c) and axial particle velocity (d) for uniform and non-uniform inlet conditions, \( Z = 3.8 \, \text{m} \).
Appendix E: Turbulence Model

The turbulence model used in chapter 3 is summarized in this section for the primary phase (gas) and the secondary phase (particles).
### Table E.1: Turbulence in primary phase

<table>
<thead>
<tr>
<th>Description</th>
<th>Equation</th>
</tr>
</thead>
</table>
| **Turbulent kinetic energy** | \[
\frac{\partial}{\partial t} \left( \alpha_g \rho_g k_g \right) + \nabla \cdot (\alpha_g \rho_g \vec{u}_g \cdot \vec{k}_g) = \nabla \cdot \left( \alpha_g \frac{\mu_{t,g}}{\sigma_k} \nabla k_g \right) + \alpha_g G_{k,g} - \alpha_g \rho_g \varepsilon_g + \alpha_g \rho_g \Pi_{k,g}
\]  
(E.1) |
| **Dissipation energy**     | \[
\frac{\partial}{\partial t} \left( \alpha_g \rho_g \varepsilon_g \right) + \nabla \cdot (\alpha_g \rho_g \vec{u}_g \cdot \nabla \varepsilon_g) = \nabla \cdot \left( \alpha_g \frac{\mu_{t,g}}{\sigma_\varepsilon} \nabla \varepsilon_g \right) + \alpha_g \frac{\varepsilon_g}{k_g} \left( C_{1e} G_{k,g} - C_{2e} \rho_g \varepsilon_g \right) + \alpha_g \rho_g \Pi_{\varepsilon,g}
\]  
(E.2) |
| **Related Equations**      | \[
\Pi_{k,g} = \sum_{s=1}^{n} \frac{K_{sg}}{\alpha_g \rho_g} \left( k_{sg} - 2k_g + \vec{v}_{sg} \cdot \vec{v}_{dr} \right)
\]  
(E.3) |
|                           | \[
\Pi_{\varepsilon,g} = C_{3e} \frac{\varepsilon_g}{k_g} \Pi_{k,g}
\]  
(E.4) |
|                           | \[
\mu_{t,g} = \rho_g \frac{C_\mu k_g^2}{\varepsilon_g}
\]  
(E.5) |
|                           | \[
G_k = -\rho_g \overline{\vec{u}_i' \vec{u}_j'} \frac{\partial \vec{u}_j}{\partial x_i}
\]  
(E.6) |

**Model constants**  
- \( C_\mu = 0.09 \),  
- \( \sigma_k = 1 \),  
- \( \sigma_\varepsilon = 1.3 \),  
- \( C_{1e} = 1.44 \),  
- \( C_{2e} = 1.92 \),  
- \( C_{3e} = 1.2 \),  
- \( C_V = 0.5 \)
Table E.2: Turbulence in secondary phase

<table>
<thead>
<tr>
<th>Equation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(E.7)</td>
<td>$k_s = k_g \left( \frac{b^2 + \eta_{sg}}{1 + \eta_{sg}} \right)$</td>
</tr>
<tr>
<td>(E.8)</td>
<td>$\eta_{sg} = \frac{\tau_{t,sg}}{\tau_{f,sg}}$</td>
</tr>
<tr>
<td>(E.9)</td>
<td>$\tau_{t,sg} = \frac{\tau_{t,g}}{\sqrt{1 + C_\beta \rho_s^2}}$</td>
</tr>
<tr>
<td>(E.10)</td>
<td>$\tau_{t,g} = \frac{3}{2} C_\mu \frac{k_g}{\varepsilon_g}$</td>
</tr>
<tr>
<td>(E.11)</td>
<td>$C_\beta = 1.8 - 1.35 \cos^2 \theta$</td>
</tr>
<tr>
<td>(E.12)</td>
<td>$\zeta = \frac{</td>
</tr>
<tr>
<td>(E.13)</td>
<td>$L_{t,sg} = \frac{3}{2} C_\mu \frac{k_g^{3/2}}{\varepsilon_g}$</td>
</tr>
<tr>
<td>(E.14)</td>
<td>$\tau_{f,sg} = \alpha_s \rho_s K_{sg} \left( \frac{\rho_s}{\rho_g} + C_V \right)$</td>
</tr>
</tbody>
</table>
Appendix F:
Steady State Condition

The appendix describes the procedure used to confirm that the model has reached the quasi steady state condition.
APPENDIX

Steady State Condition

The multiphase flow in CFB riser is chaotic and transient. Therefore reaching an exact steady state condition is not possible. However a quasi steady state condition can be reached when the riser contains the desired particle loading. In the present work the quasi steady condition was confirmed by monitoring the solid mass flux at the outlet. The integration of solid mass flux over the outlet cross section gave an average solid mass flux of 462 kg/m²s, which is 1.6% different from the inlet solid flux value (455 kg/m²s) after 15 s from the beginning of the simulation, and then fluctuated with ± 2.2% of the inlet solid flux value. This indicates that the quasi steady state condition was reached after 15 s.
Fig. F.1: Transient behavior of the integral solid mass flux at the riser outlet.