Numerical Investigation to Study the Segregation Characteristics in Fluidized Bed Gasifiers

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To my very Supportive Loving and Caring

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All acclaim and eminence be to "ALLAH", a definitive creator of this universe, who endowed us with the ability to comprehend and made us curious to investigate this entire universe. Infinite greetings upon the leader of this universe and hereafter "HOLY PROPHET HAZRAT MUHAMMAD (PBUH)": the wellspring of beneficial information and blessings for the whole humankind and Uma.

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Muhammad Haseeb Iqbal

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CFD	Computational Fluid Dynamics
TFM	Two Fluid Model Theory
KGTF	Kinetic Theory of Granular Flow
GUI	Graphical User Interface

ABSTRACT

In this work, the flow properties of gas-solid fluidized beds are investigated, with particular attention to Geldart-B particles that differ in size but have comparable densities, as well as particles that have the same size but variable densities. The investigation explores the impact of various factors on bed behavior, including bed dimensions, gas velocity profiles, initial bed height, solid fraction variations, and particle properties such as density, restitution coefficient, and specularity coefficient. It also assesses the impact of mesh size on computational accuracy and evaluates different drag models for their effectiveness in simulating fluidized bed dynamics. The simulation framework is validated against real data from experiments, ensuring that simulated results closely match real-world observations and enhancing the model's reliability. Combining experimental data with simulations confirms the theoretical framework and improves models' predictive capabilities. The integrated approach provides insights into optimizing fluidized bed operations for various industrial applications. Understanding the interaction of factors like particle size, density, and bed geometry allows for adjustments in operational parameters, enhancing efficiency and performance. Accurate predictions aid in designing and scaling up fluidized bed systems with greater confidence. This research advances the understanding and predictive accuracy of gas-solid fluidized bed systems, providing a strong foundation for further exploration and optimization of these technologies, supporting innovation and improvement in related industrial processes.

Keywords: Gas Solid Fluidized Bed, Size segregation, Density Segregation, Geldart B.

CHAPTER 1. INTRODUCTION

1.1. Background and Context

Many industrial operations extensively use Gas-solid fluidization, which includes power production and petrochemical conversion processes. The primary benefits of fluidization include its capacity to efficiently handle solid materials and maintain isothermal conditions through excellent solid mixing facilitated by a high surface area. [1].

The quality of fluidization is strongly influenced by the inherent qualities of particles, such as density, size, distribution, and surface characteristics of particles. [2]

Industrial application of fluidization usually has solid particles with different size and density, this change in properties results in a phenomenon known as segregation which occurs when fluidization is done with low velocity.[3]. In a fully fluidized bed bubbles form and distribute the particles across the bed. Bubbles create a wake and drift, which mixes and segregates the particles.[4] The particles that are collected at the top of the bed are known as flotsam and those that accumulate at the bottom are known as jetsam.[5] Denser particles tend to settle down (jetsam) in a system where density is the key difference between particles fluidized together.[3]

Fine particles, typically used in industrial fluidization applications, fall into four distinct groups. Geldart group A particles exhibit excellent fluidization behavior, characterized by a smooth expansion without bubble formation. Geldart groups B or D exhibit minimal bed expansion during fluidization. Due to their high cohesion, Geldart group C particles exhibit poor fluidization.[6] This study focuses solely on Geldart B-type particles.

Various modeling tools have been employed to investigate the complex behavior of fluidization. The two-fluid model, or Eulerian method, is employed for small scale setups [7] due to its less computational cost as compared to large industrial setups [8]. For large industrial scale setups TFM requires fine meshing and detailed explanation of gas-solid interactions for momentum exchange between the phases. Irrespective of its detailed input for industrial setups TFM is widely used for hydrodynamic prediction of industrial setups.[9], [10] The local averaged quantities in the two-fluid model are obtained by averaging the local quantities in the gas and solid phases of TFM by averaging across the microscopic conservation equations. Even though flow details at the element level are eliminated and the discontinuities between two phases are smoothed through averaging, their impacts manifest in the averaged equations through important relations such as drag force and solid stress. The main objective of this study is to select a validate a drag model that will predict the hydrodynamic behavior accurately for varying density and same size, varying sizes and same density systems.

CFD is a promising tool to predict the behavior of single-phase flow and multiphase phase flow, but the validation and verification of multiphase phase flow for different applications require improvement and further testing for fluidized beds gasifiers. [11]

1.2. Problem Statement

This work aims to validate an experimental model incorporating identically sized particles with various densities and particles with comparable densities but different sizes. Comparing simulation models with experimental data that incorporates various drag models will be part of the validation process.

1.3. Research Objectives and Questions

Developing a CFD technique to precisely forecast the hydrodynamics of gas-solid fluidized beds is the main goal of this thesis. To accomplish this overall objective, the subsequent particular research inquiries will be tackled:

1. How can we integrate CFD techniques to improve the predictive accuracy of fluidized bed hydrodynamics models?
2. What optimization techniques can be effectively applied to enhance the performance of the CFD model?

1.4. Significance and Motivation

The successful development of a CFD model can have significant implications for the field of fluidized bed research and industrial applications.

This research holds the potential to:

- Improve the accuracy and efficiency of predicting fluidized bed hydrodynamics, leading to more effective process optimization.
- Reduce the reliance on costly experimental studies, saving time and resources.
- Enable better understanding and control of fluidized bed systems in various industrial processes, contributing to improved sustainability and environmental performance.

1.5. Scope and Limitations

With a focus on Geldart-B particles, this study will construct a CFD model to forecast the hydrodynamics of gas-solid fluidized beds. The behavior of binary particle mixes in fluidized beds will be the focus of the investigation. These are some of the research's limitations:

1. The study's findings may not be directly transferable to all fluidized bed systems due to variations in particle properties and operating conditions.
2. The performance of the CFD model may depend on the quality and quantity of available data.

1.6. Organization of Thesis

The remaining sections of this thesis are arranged as follows:

- Chapter 2 will provide relevant literature on Fluidized bed gasification and computational fluid dynamics (CFD) modelling.
- Chapter 3 outlines the theoretical framework and working principles of CFD.
- Chapter 4 outlines the methodology
- Chapter 5 presents the results and discussions.

CHAPTER 2. LITERATURE REVIEW

2.1 Literature Review

Fluidization refers to the process of transforming a bed of solid particles into a state resembling a liquid. This is accomplished by directing a gas or liquid against the force of gravity through the bed. Fluidization has been utilized commercially for over a century and has been used in various processes such as drying, adsorption, fluid catalytic cracking, gasification, pyrolysis, and more. The primary benefits of fluidization are enhanced heat transfer, effortless mobility of solids akin to liquids, and the capacity to handle a diverse variety of particle sizes. The temperature of the fluidized bed can be consistently controlled within a narrow range, even during highly exothermic reactions[12], [13].

This intricate procedure is utilized in diverse industries, including refineries, where it is employed to transform low-octane fuel into high-octane fuel in a fluid catalytic cracker. This method encompasses several configurations based on factors such as length, flow, transport qualities, and feed alterations. This intricate procedure necessitates optimization at both the reactor level and the micro scale, where each individual particle actively contributes to the whole process[14]. Understanding the entirety of fluidization necessitates a thorough grasp of the subject, which may be attained through precise and all-encompassing simulation. This simulation is crucial for the design, operation, and optimization of industrial processes.

Computational fluid dynamics models have facilitated the comprehension of the gas-solid interactions occurring during fluidization processes. Computational Fluid Dynamics (CFD) is a reliable method for accurately predicting the mixing efficiency and temperature profiles of solid and gaseous phases. This enables the optimization of the design and operation of fluidized bed installations. Gas and solid flow in CFD modelling are dependent on Eulerian-Eulerian and Eulerian-Lagrangian approaches.

In Lagrangian approach, equations are solved for individual particle which gives better understanding of mixing and segregation phenomena, but the constraint of its application for number of particles (typically < 106) limit its application to coarse particles only.[15]

In Eulerian-Eulerian approach two fluid model which is based on Kinetic Theory of Granular Flow (KGTF) is also used for simulating the gas solids flow[16]. The TFM model describes gas and solid phase as an individual continuous phase which are interpenetrating into each other and for computation of solid phase KGTF is employed, this interpenetrating effect of fluids is accurately explained using drag models [17], [18]. Accurate result calculations also depend on the selection of suitable boundary conditions.

The selection of Eulerian-Eulerian or Eulerian-Lagrangian approach depends on nature of application for which they are employed. The later one should be applied to a binary or poly-disperse system while first one shall be applied to the complex geometries.

The two fluid model approach describes gas and solid phase as an interpenetrating continuum, and to calculate kinetic theory of granular flows is used to compute solid phase characteristics. Ensuring accurate predictions with the TFM approach hinges on judicious model selection and the application of suitable boundary conditions to capture gas-solid interactions. Notably, gas-solid flow exhibits aggregative behavior, resulting in heterogeneous structures across varying time and spatial scales. For instance, in gas-solid fluidized beds, flow structures evolve in response to material properties and operational conditions. To model this behavior, it is common to treat the statistical behavior of numerous particles with similar diameters and densities as approximating a continuum with continuous density and velocity distributions. This hydrodynamic model is widely recognized as the two-fluid model (TFM) and finds extensive application in industrial simulations found in the literature. In recent years CFD research shown that TFM is accurately predicting the hydrodynamic behavior of Geldart B particles. [17], [19]

In fluidized bed system, particles tend to settle according to size and density, leading to distinct distributions within the bed. This segregation affects the bed's flow dynamics, stability, and heat/mass transfer characteristics. Researchers, including [20], have investigated how above-mentioned factors result in the formation of segregated clusters or layers within the bed, influencing gas-solid mixing and residence time. Validating hydrodynamics models is essential to understand and predict segregation accurately. For example, [21] investigated how particle size ratios affect mixing and segregation, while [21] and [15] explored the flow behavior and segregation kinetics. Additionally, [22] used simulations to study particle distribution. Conditions at wall also dictate the simulation results, this was found by the study done by [23]. The specularity coefficient is also governs the simulation results which was highlighted by [24], [25], [26]. The restitution coefficient in an input for KGTF based models at accounts for particle-particle collisions, different researchers have contributed for selection of its value, [27] reported that criticality of restitution coefficient is diminishes after a certain value and it remain sensitive between 0.6 -0.99. This comprehensive understanding of segregation and model validation is crucial for optimizing fluidized system design and operation across various industries, ensuring efficient and effective processes. Furthermore, the impact of segregation extends to powder handling systems, where it influences processes such as powder mixing. Understanding segregation phenomena in these systems is essential for achieving uniform powder distribution and preventing issues like particle segregation during blending. Researchers have investigated segregation mechanisms in powder handling systems to develop strategies for minimizing segregation effects. Studies by [28] and [29] have explored the factors affecting segregation during powder mixing, providing insights into the design of equipment and process parameters to mitigate segregation. Moreover, segregation can occur among particles of the same size but with different densities, as well as particles of the same density but with different sizes, further complicating system behavior and requiring careful consideration in process design and optimization efforts. By addressing segregation challenges in both fluidized bed reactors and powder handling systems, industries can enhance product quality, reduce waste, and improve overall process efficiency.

In their research, [30] used an Eulerian-Eulerian model in a two-dimensional domain to investigate the link between size of solid particles and the effect of surface velocity on bubbling fluidized beds. The CFD model's bed expansion and bed pressure drop results were found to closely match the experimental findings, demonstrating the model's ability to faithfully replicate actual experimental results. [31] studied and simulated the impacts of several drag models. Gidaspow and Syamlal-Obrien, two widely used drag models, were investigated in the investigation of bubbling fluidized beds simulation. The results showed that, in comparison to the experimental data, both simulation models produced outcomes that were comparable. Nonetheless, the

Syamlal-Obrien model demonstrated the trend that was most similar to the experimental data when comparing bubble probability. The impacts of the drag function, granular temperature, turbulence model, frictional stress model, and discretization scheme with various distributors and slotted draft tubes were examined in [32].

CHAPTER 3. THEORETICAL FRAMEWORK

3.1 Principle of Gas Solid Fluidized Bed

3.1.1 Working principle of fluidized beds

A fluidized bed consists of solid particles (typically a granular material) suspended and mixed with a gas or liquid flow in such a way that it behaves like a fluid. The bed appears to be bubbling and swirling, with the solid particles exhibiting fluid-like behavior, such as mobility and a lack of distinct boundaries.

The key working principles of fluidized beds include:

Fluidization: The process begins with a bed of solid particles placed inside a container or chamber. A fluidizing medium, usually a gas (e.g., air or nitrogen) or a liquid (e.g., water), is introduced from the bottom of the bed. As the fluidizing medium flows upward through the bed, it imparts enough energy to the solid particles to overcome gravity, causing them to become suspended and exhibit fluid-like properties.[27]

Minimum Fluidization Velocity (Umf): Velocity of the fluid at which the drag forces acting on the fluid (solid particles) is balanced by the force of gravity, this velocity is called Minimum Fluidization Velocity (Umf)[33], the particles settle and form a packed bed. At Umf, the particles start to become suspended and gently fluidized.

Bubbling and Turbulent Fluidization: The bed enters the bubbling fluidization regime, which is marked by the development of bubbles that rise through the bed, when the velocity increases beyond Umf. It enters a turbulent fluidization zone at higher velocities, characterized by severe mixing and bubbling[34].

Uniform Mixing and Heat Transfer: Fluidized beds provide excellent mixing of solid particles with the fluidizing medium, leading to uniform temperature and concentration distributions. This uniformity enhances heat transfer and mass transfer, making fluidized beds ideal for various chemical reactions and heat exchange processes.[35]

3.1.2 Components of fluidized bed system

A typical fluidized bed system consists of the following components:

Bed Material: Inside the fluidized bed is this solid substance. It could be any granular material appropriate for the intended process, such as sand in a heat exchanger or catalyst particles in a chemical reactor.

Fluidizing Medium: The fluidizing medium can be a gas (e.g., air or nitrogen) or a liquid (e.g., water). It is introduced from the bottom of the bed and is responsible for suspending and fluidizing the solid particles.

Distributor/Plenum: The distributor is the structure at the bottom of the fluidized bed that evenly distributes the fluidizing medium across the bed's cross-section. It may consist of nozzles or perforated plates.

Gas/Liquid Inlet: This is the point at bed where the fluidizing medium is introduced into the bed.

Outlet: The outlet allows the fluidizing medium and any products or particles to exit the bed.

Heat Exchanger or Reactor: The fluidized bed reactor or heat exchanger is the main processing unit where chemical reactions, heat transfer, or other processes occur.

3.1.3 Applications of Fluidized Beds

Fluidized beds find applications in various industries, including:

Chemical Industry: Fluidized bed reactors are used for catalytic cracking, polymerization, and fluidized bed combustion for chemical production.

Pharmaceutical Industry: They are employed for drying, granulation, and coating of pharmaceutical particles.

Food Industry: Fluidized beds are used in food drying, frying, and coating processes.

Energy Production: Fluidized bed combustion is utilized in power plants for efficient coal and biomass combustion, reducing emissions.

Environmental Engineering: Fluidized bed systems can be employed for waste incineration and wastewater treatment.

Metallurgical Industry: They are used in ore roasting, calcination, and particle coating processes.

3.1.4 Advantages of Fluidized Beds

Fluidized beds offer excellent mixing and stable temperature distribution, along with rapid mass and heat transmission rates. They enhance reaction kinetics, making them suitable for catalytic reactions, and provide good control over process parameters. Additionally, fluidized beds contribute to reduced emissions in combustion processes due to lower combustion temperatures.

3.1.5 Disadvantages and Challenges

The design and operation of fluidized beds can be complex, requiring careful consideration of parameters like particle size and gas velocity. Abrasion and attrition of particles can lead to equipment wear, and there is a potential for elutriation (particle entrainment) in high gas velocity conditions. Additionally, temperature control and maintenance can be challenging.

3.1.6 Geldart's Classification

Geldart's [36] classification distinguishes four main groups of solid particles:

1. Group A: Geldart Group A particles are fine and cohesive powders that tend to agglomerate when fluidized. They exhibit poor fluidization behavior and can lead to bed defluidization due to excessive particle-particle interactions. Examples of Group A particles include fine clays and cohesive powders.

2. Group B: Group B particles are non-cohesive and exhibit good fluidization characteristics. They maintain stable fluidization even at high gas velocities. Sand and most commonly used catalyst particles in fluidized bed reactors fall into this category.

3. Group C: Group C particles are characterized by their fine size and the tendency to form bubbles in the bed. These bubbles can lead to non-uniform fluidization

and mixing. Examples of Group C particles include fine powders like alumina.

4. Group D: Geldart Group D particles are coarse and non-cohesive. They have limited fluidization potential and tend to behave as static beds, only showing minimal expansion. Grains, granules, and certain ores are typical examples of Group D particles.

3.1.7 Fluidization Regimes

There are various fluidization regimes in which gas-solid fluidized beds can exist, including:

The Minimum Fluidization Velocity (Umf) is the specific velocity of the fluid at which the bed of particles begins to fluidize, marking the threshold where the particles are lifted and start to behave like a fluid. When the velocities are just above Umf, the bed enters a state known as a Partly Fluidized Bed. In this state, the bed is only partially fluidized, meaning that some particles are lifted and fluidized while others remain stationary and settled at the bottom. As the velocity continues to increase beyond this point, the bed transitions into a state of Turbulent Fluidization. This higher velocity state is characterized by vigorous mixing of the particles and significant bed expansion, leading to more dynamic interactions within the fluidized bed.

Understanding these regimes and Geldart's classification is essential for designing and operating fluidized bed reactors effectively.

3.2 Fundamentals of CFD

3.2.1 Introduction to CFD

Gas fluidized bed simulation can be done via (CFD) to understand fluid flow and heat transfer phenomena. CFD allows engineers and researchers to gain insights into the interactions between solid and gas particles, aiding in the design and optimization of fluidized bed processes. The fundamentals of CFD are rooted in the Navier-Stokes equations, which describe fluid flow behavior.

3.2.2 Governing Equations

The Navier-Stokes equations, comprising the continuity equation and the momentum equation, are central to CFD simulations. These equations govern the conservation of mass and momentum within a fluid domain. Additionally, the energy equation accounts for heat transfer processes. Researchers commonly employ numerical methods like finite difference, finite element, or finite volume methods to discretize and solve these equations. The governing and constitutive equations are given in tables Table 3.1 and Table 3.2 respectively.

Table 3.1: Governing Equations

Equations	**Mathematical expressions**
Mass conservation equations of gas and solids phases	$\frac{\partial(\alpha_g\rho_g)}{\partial t} + \nabla\cdot\left(\alpha_g\rho_g\vec{u}_g\right) = 0$ Eq-1 $\frac{\partial(\alpha_s\rho_s)}{\partial t} + \nabla\cdot(\alpha_s\rho_s\vec{u}_s) = 0$ Eq-2 $\alpha_g + \alpha_s = 1$ Eq-3
Momentum conservation equations of gas and solids phases	$\frac{\partial(\alpha_g\rho_g\vec{u}_g)}{\partial t} + \nabla\cdot\left(\alpha_g\rho_g\vec{u}_g\vec{u}_g\right) = \nabla\cdot\left(\bar{\bar{\tau}}_g\right) - \alpha_g\nabla P - \beta\left(\overrightarrow{u_g}\overrightarrow{u_s}\right) + \alpha_g\rho_g g$ Eq-4 $\frac{\partial(\alpha_s\rho_s\vec{u}_s)}{\partial t} + \nabla\cdot(\alpha_s\rho_s\vec{u}_s\vec{u}_s) = \nabla\cdot\left(\bar{\bar{\tau}}_g\right) - \alpha_s\nabla P - \beta\left(\overrightarrow{u_g}\overrightarrow{u_s}\right) + \alpha_s\rho_s g$ Eq-5
Granular Temperature	$\Theta = \frac{1}{3}u'^2$ Eq-6
Equation of conservation of solids fluctuating energy	$\frac{3}{2}\left(\frac{\partial(\alpha_s\rho_s\Theta)}{\partial t} + \nabla\cdot(\alpha_s\rho_s\vec{u}_s\Theta)\right) = \left(-P_s\bar{\bar{I}} + \bar{\bar{\tau}}_s\right):\nabla\vec{u}_s - \nabla\cdot q - \gamma - J$ Eq-7

Table 3.2: Constitutive Equations

Equations	Mathematical expressions
Gas phase stress tensor [37]	$\bar{\tau}_g = \alpha_g \left[\left(\xi_g - \frac{2}{3}\mu_g \right) (\nabla \cdot \vec{u}_g) I + \mu_g \left((\nabla \vec{u}_g) + (\nabla \vec{u}_g)^T \right) \right]$
Solid phase stress tensor [37]	$\bar{\bar{\tau}}_s = -\alpha_s \left[\left(\xi_s - \frac{2}{3}\mu_s \right) (\nabla \cdot \vec{u}_s) \bar{\bar{I}} + \mu_s \left((\nabla \vec{u}_s) + (\nabla \vec{u}_s)^T \right) \right]$
Solids pressure [37]	$P_s = \alpha_s \rho_s \Theta + 2 g_0 \alpha_s^2 \rho_s \Theta (1 + e_s)$
Solids shear viscosity	$\mu_s = \mu_{s,col} + \mu_{s,kin} + \mu_{s,fr}$
Collisional viscosity [38]	$\mu_{s,\mathrm{col}} = \frac{4}{5} \alpha_s \rho_s d_s g_0 (1 + e_s) \sqrt{\frac{\Theta}{\pi}}$
Kinetic viscosity [38]	$\mu_{s,kin} = \frac{10}{96} \sqrt{\Theta \pi} \frac{\rho_s d_s}{(1 + e_s) \alpha_s g_0} \left[1 + \frac{4}{5} g_0 \alpha_s (1 + e_s) \right]^2$
Kinetic viscosity [39]	$\mu_{s,k\,\mathrm{in}} = \frac{\alpha_s \rho_s d_s \sqrt{\theta \pi}}{6(3 - e_s)} \left[1 + \frac{2 \sim}{5} g_0 \sim \alpha_s \sim (1 + e_s)(3 e_s - 1) \right]$
Frictional viscosity [40]	$\mu_{s.ff} = \frac{P_s \sin \phi}{2\sqrt{l_{2p}}}$

Frictional viscosity [41]	$P_{\text{friction}} = Fr\frac{(\alpha_s - \alpha_{s,\min})^n}{(\alpha_{s,\max} - \alpha_s)^p}$
Solids bulk viscosity [37]	$\xi_s = \frac{4}{3}\alpha_s\rho_s d_s g_0(1 + e_s)\sqrt{\frac{\theta}{\pi}}$
Radial distribution function [37]	$g_0 = \left[1 - \left(\frac{\alpha_s}{\alpha_{\sin}}\right)^{1/3}\right]^{-1}$
Collisional energy dissipation [37]	$\gamma_s = 3(1 - e_s^2)\alpha_s^2\rho_s g_0\Theta\left(\frac{4}{d_e}\sqrt{\frac{\Theta}{\pi}}\right)$

3.2.3 Modelling of Gas-Solid Flows

This section covers the modeling of gas-solid flows within gas-solid fluidized beds using the TFM, the Eulerian-Eulerian approach, and associated ideas such as drag modeling and KTGF.

Eulerian-Eulerian Approach:

The Eulerian-Eulerian approach treats the gas and solid phases as interpenetrating continua, each having its set of conservation equations[42]. In this approach:

The gas phase in fluidized bed systems is accurately described by the Navier-Stokes equations, which include the continuity, momentum, and energy equations, as discussed earlier. These equations provide a comprehensive framework for understanding the behavior of the gas phase, capturing the essential dynamics of flow, pressure, and thermal energy transfer. Similarly, the solid phase is described using a parallel set of equations that consider the specific properties of the solid particles. These equations take into account the unique density, velocity, and energy characteristics of the solids, allowing for a detailed and precise depiction of their behavior within the fluidized bed system. By employing these detailed mathematical models for both the gas and solid phases, the complex interactions and overall dynamics of fluidized beds can be thoroughly understood and accurately predicted.

The interaction between the gas and solid phases is represented through various modeling techniques, such as drag models and interphase heat transfer models. These models account for the forces and heat transfer between the two phases. Key points to consider in the Eulerian-Eulerian approach include:

Interphase drag refers to the drag force exerted by the solid particles on the gas phase and vice versa, and it is crucial for accurate modeling of fluidized beds. Various drag models, such as the drag coefficient and friction factor models, can be employed to capture this interaction effectively [43]. Additionally, interphase heat transfer between the gas and solid phases is vital for accurately capturing the temperature distribution within the fluidized bed. This aspect is especially important when studying reactions involving solid particles, as it significantly influences the thermal dynamics and overall efficiency of the reactions.

3.2.4 Two-Fluid Model (TFM):

The Two-Fluid Model (TFM) is a widely used approach for simulating gas-solid flows in fluidized beds. It considers two interpenetrating continua: the gas phase and the solid phase.[44] In TFM:

Each phase in a fluidized bed system has its own set of conservation equations, which include continuity, momentum, and energy equations. These equations describe the fundamental principles of mass, force, and thermal energy conservation for both the gas and solid phases. The interaction between these phases is captured through source terms in the momentum and energy equations, which represent the effects of drag forces and heat transfer between the gas and solid phases. These source terms are essential for coupling the phases, as they account for the transfer of momentum due to drag forces and the exchange of thermal energy, thereby linking the behavior of the gas phase with that of the solid phase in a comprehensive and accurate manner.

Key features of TFM include:

In the Two-Fluid Model (TFM) for fluidized bed systems, volume fractions are employed to represent the proportion of each phase present in a given control volume. These volume fractions are crucial for calculating mass and momentum exchange terms between the gas and solid phases. To describe the interactions between these phases, TFM often relies on empirical drag models, with commonly used models including the Schiller-Naumann and Gidaspow models. These drag models provide a means to quantify the forces exerted between the gas and solid particles. Additionally, heat transfer between the phases is represented using heat transfer coefficients that account for both conduction and convection processes. These coefficients are essential for capturing the thermal interactions between the gas and solid phases, which play a significant role in the overall dynamics and efficiency of the fluidized bed system.

In summary, both the Eulerian-Eulerian approach and the Two-Fluid Model (TFM) are valuable tools for modeling gas-solid flows within fluidized beds. These approaches allow researchers and engineers to gain insights into the complex interactions occurring within fluidized beds and are essential for the design and optimization of processes in various industries. Properly chosen models and accurate parameter estimation are critical for obtaining reliable simulation results.

3.2.5 Drag Models

In the realm of CFD simulations for fluidized beds, it becomes imperative to elucidate the interplay between particles and the transfer of momentum between distinct phases. This interaction, particularly between particles and the continuous gas phase, is encapsulated by drag models, and various models have been developed for this explicit purpose. These models intricately capture the momentum exchange occurring between the phases, with drag standing out as a pivotal term within the granular phase's momentum equation. The selection of different drag models holds substantial influence over the dynamics of the granular phase, exerting discernible effects on predicted bed expansion and particle concentration within the bed's densely populated regions. The ensuing section outlines the equations integral to the drag models employed in this study.

Gidaspow

The Ergun Eq. and Wen-Yu Model are combined to create the Gidaspow model [45]. In this drag model, the interphase momentum exchange coefficient K_{gp} is specified as follows:

Ergun equation:

$$K_{\mathrm{gp-\,Ergun}} = 150\frac{\varepsilon_{\mathrm{p}}(1-\varepsilon_{\mathrm{g}})\mu_{\mathrm{g}}}{\varepsilon_{\mathrm{g}} d_{\mathrm{p}}^{2}} + 1.75\frac{\rho_{\mathrm{g}}|\boldsymbol{v}_{\mathrm{p}}-\boldsymbol{v}_{\mathrm{g}}|}{d_{\mathrm{p}}}, \varepsilon_{\mathrm{g}} \leq 0.80$$

Wen-Yu model:

$$K_{\mathrm{gp}-WenYu} = \frac{3}{4}C_{\mathrm{d}}\frac{\varepsilon_{\mathrm{p}}\varepsilon_{\mathrm{g}}\rho_{\mathrm{g}}|\boldsymbol{v}_{\mathrm{p}}-\boldsymbol{v}_{\mathrm{g}}|}{d_{\mathrm{p}}}\varepsilon_{\mathrm{g}}^{-2.65},\ \varepsilon_{\mathrm{g}} > 0.80$$

where, $|\boldsymbol{v}_{\mathbf{p}}-\boldsymbol{v}_{\mathbf{g}}|$ is the slip velocity and C_{d} is the drag coefficient. The drag coefficient C_d can be defined as follows:

$$C_{\mathrm{d}} = \begin{cases} \dfrac{24}{\varepsilon_{\mathrm{g}R} Re_{\mathrm{p}}}\left[1+0.15\left(\varepsilon_{\mathrm{g}R} Re_{\mathrm{p}}\right)^{0.687}\right] & ,\mathrm{Re}_{\mathrm{p}} < 1000 \\ 0.44, & Re_{\mathrm{p}} \geq 1000 \end{cases}$$

Syamlal-O'Brien model

Equations based on the volume fraction and relative Reynolds number are used to calculate the terminal velocity of the particles in fluidized or settling beds, which forms the basis of this model. For this drag model, the interphase momentum exchange coefficient, K_{gp} has the following definition:

$$K_{\mathrm{gp-\,Syamlal\text{-}O,Brien}} = \frac{3\varepsilon_{\mathrm{p}}\varepsilon_{\mathrm{g}}\rho_{\mathrm{g}}}{4v_{\mathbf{r},\mathrm{p}}^{2} d_{\mathrm{p}}} C_{\mathrm{d}}\left(\frac{Re_{\mathrm{p}}}{v_{\mathbf{r,p}}}\right)|v_{\mathbf{p}}-v_{\mathrm{g}}|$$

$$v_{\mathbf{r,p}} = 0.5\left(A - 0.06\mathrm{Re}_{\mathrm{p}} + \sqrt{\left(0.06\mathrm{Re}_{\mathrm{p}}\right)^{2} + 0.12\mathrm{Re}_{\mathrm{p}}\,(2B-A) + A^{2}}\right)$$

with $A = \varepsilon_{\mathrm{g}}^{4.14}$ and $B = 0.8\varepsilon_{\mathrm{g}}^{1.28}$ for $\varepsilon_{\mathrm{g}} \leq 0.85$ and $B = \varepsilon_{\mathrm{g}}^{2.56}$ for $\varepsilon_{\mathrm{g}} > 0.85$.

The KGTF is used to simulate the constitutive equations for the solid stress tensor $(\boldsymbol{\tau}_{\mathbf{p}})$ in the TFM [45].

$$\boldsymbol{\tau}_{\mathbf{p}} = -p_{\mathrm{p}}\boldsymbol{I} + \varepsilon_{\mathrm{p}}\mu_{\mathrm{p}}\left(\nabla\boldsymbol{v}_{\mathbf{p}} + \nabla\boldsymbol{v}_{\mathbf{p}}{}^{T}\right) + \varepsilon_{\mathrm{p}}\left(\lambda_{\mathrm{p}} - \frac{2}{3}\mu_{\mathrm{p}}\right)\nabla\cdot\boldsymbol{v}_{\mathbf{p}}\boldsymbol{I}$$

Wen-Yu model

The interphase momentum exchange coefficient, K_{gp} in the Wen-Yu model is defined as follows:[46]

$$K_{\mathrm{gp-\,WenYu}} = \frac{3}{4}C_{\mathrm{d}}\frac{\varepsilon_{\mathrm{p}}\varepsilon_{\mathrm{g}}\rho_{\mathrm{g}}\left|\boldsymbol{v}_{\mathrm{p}} - \boldsymbol{v}_{\mathrm{g}}\right|}{d_{\mathrm{p}}}\varepsilon_{\mathrm{g}}^{-2.65}$$

where C_d is the drag coefficient which can be defined as follows:

$$C_{\mathrm{d}} = \frac{24}{\varepsilon_{\mathrm{g}}Re_{\mathrm{p}}}\left[1 + 0.15\left(\varepsilon_{\mathrm{g}}Re_{\mathrm{p}}\right)^{0.687}\right]$$

3.2.6 Kinetic Theory of Granular flow (KTGF)

The kinetic theory of granular flow provides a framework for understanding the behavior of collections of macroscopic particles, such as sand or powders. In this theory, granular materials are treated as many individual particles as possible with distinct velocities and interactions. Unlike the continuous flow of gases in the kinetic theory of gases, granular materials exhibit discrete, collision-dominated behavior. The theory focuses on the interplay between particle collisions, dissipative forces, and the transfer of kinetic energy. Granular flows often display intriguing phenomena like segregation and clustering, challenging the traditional fluid dynamics approaches. Understanding granular dynamics is vital in industries ranging from agriculture to pharmaceuticals, as well as in natural processes like landslides. The kinetic theory of granular flow not only aids in predicting and controlling these materials' behavior but also contributes to advancements in fields requiring the handling and processing of granular substances [4].

CHAPTER 4. METHODOLOGY

4.1. Data Collection and Analysis

- Gather experimental data from the two sources mentioned: one set with particles of the same size but different densities, and another set with particles of the same density but different sizes.
- Analyze the experimental data to understand the behavior of the particles in different conditions. This analysis should include parameters such as particle velocities, trajectories, and interactions with the fluid medium.

4.2. Model Development

- Create a computational fluid dynamics (CFD) model in Ansys Fluent.
- Eulerian-Eulerian (Two fluid model) will be applied for model development
- Define the geometry of the system, from experimental data, this includes the column geometry, initial bed height, column diameter. The geometry definition also includes the mesh size.
- Set up the fluid flow conditions, such as inlet velocity, temperature, and boundary conditions.
- Incorporate the properties of the particles into the model, including size, density, and material properties.
- Implement appropriate models for particle-fluid interactions, such as drag force, lift force, and particle-particle collisions.
- Grid independence test was conducted on different mesh sizes i.e., 5x5 and 7x7.
- Time step selection was done to incorporate the effect of time step.
- Validate the model by comparing its predictions with the experimental data from both sources separately using axial profiles, and velocity contours.

CHAPTER 5. RESULT AND DISCUSSION

CFD Results and Discussion

5.1. Experimental Setup

a b

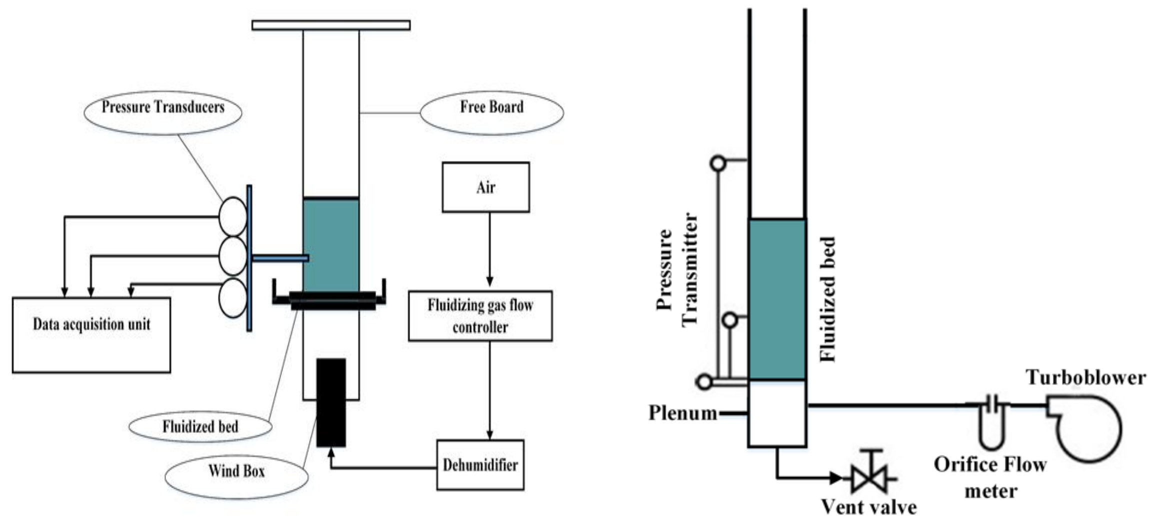

Figure 5.1: Schematics of Experimental Setup: **(a)** Marzocchella et al [47] Plexiglas Fluidization Column **(b)** Joseph et al [28] Plexiglas Fluidization Column

The experimental setup for validation that we chose for this study are given in Fig. 5.1 (a). Geometry of Marzocchella in which they used a Plexiglas column with an internal diameter of 0.12 m, and the total height of the column is 1.5m with a controller for gas flow, a dehumidifier was also used with geldart-B type particles in the column with physical properties mentioned in Table 5.1. For Joseph et al shown in Fig 5.1 (b). which also used Plexiglas column of dia 0.12m with stainless steel plate used as a distributor and geldart-B particles. The selection of numerical scheme and simulation setup is shown in Table 5.2.

Table 5.1: Physical and Operating Conditions for Marzocchella et al [47] Experimental Setup

Parameters	Values
Small particle density, ρ_{p1}, kg/m^3	2500
Small particle diameter, d_{p1}, μm	125
Large particle density, ρ_{p2}, kg/m^3	2500
Large particle diameter, d_{p2}, μm	500
Minimum fluidization velocity for small particles, U_{mf1}, m/s	0.017
Minimum fluidization velocity for large particles, U_{mf2}, m/s	0.22
Air velocity, U_g, m/s	0.09
Air density, ρ_g, kg/m^3	1.225
Air viscosity, μ_g, kg/(m·s)	1.7894×10^{-5}

Table 5.2: Simulation Settings

Relevant parameters	Marzochella Experiment
Viscous model	Laminar
Unsteady formulation	First-order implicit
Pressure-velocity coupling	Phase couple SIMPLE
Momentum discretization	Second-order upwind
Volume fraction discretization	Quick
Granular Temperature	Algebraic
Granular viscosity	Gidaspow
Granular bulk viscosity	Lun et al.
Frictional viscosity	Schaeffer
Angle of internal friction	30°
Frictional pressure	Based KTGF
Frictional packing limit	0.61
Solids pressure	Lun et al.
Radial distribution	Lun et al.
Restitution coefficient	0.9
Under relaxation factors	Default
Gas-solid drag	Gidaspow / Wen & Yu / Huilian-Gidaspow
Solid-solid drag	Syamlal-Obrien-symmetric
Time step	0.0002, 0.0005, 0.001

5.2. 2D Schematics

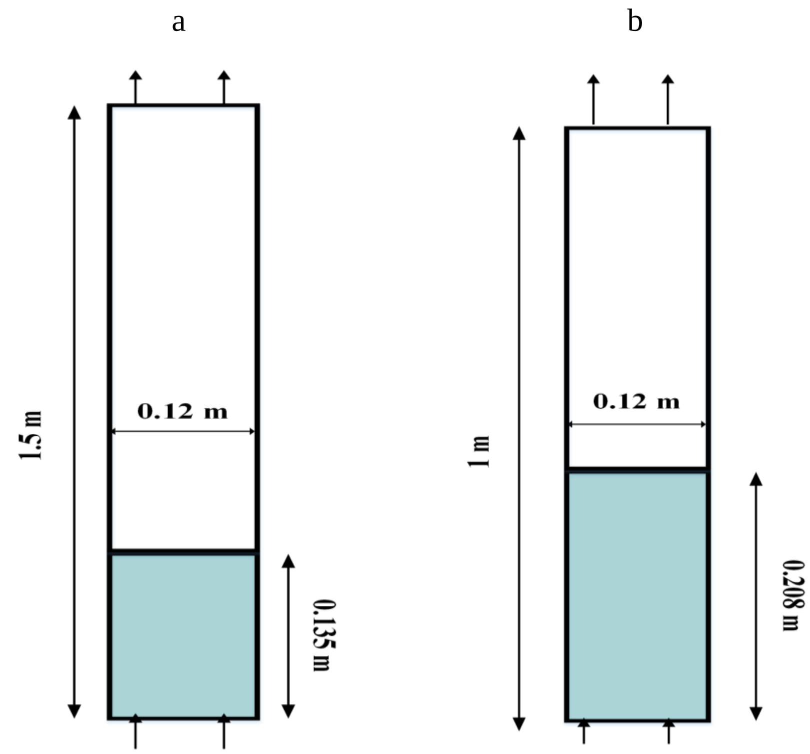

Figure 5.2: 2D Schematics of Experimental Setup of Bubbling Fluidized Bed
(a) Marzocchella et al [47] Plexiglas Fluidization Column
(b) Joseph et al [28] Fluidization Column

To demonstrate the CFD framework, a 2D schematics of a gas-solid fluidized bed reactor system from Marzocchella et al [47] is shown in Figure 5.2 (a) which has a height of 1.5 m and diameter of 0.12 m. The disengaging section was neglected to save computation time. Particles with minimum fluidization voidage are initially packed.

For the bubbling fluidized column of Joseph et al [13], the fluidized column was 1.0 m in height and 0.12 m in diameter.

5.3. Grid Independency Test

A grid independence test is a process in which different grid resolutions are examined to assess whether the numerical solution is insensitive to the mesh size, ensuring that the results are not significantly affected by the grid density. In this study, three grids with resolutions of 5 by 5, and 7 by 7 were evaluated concerning the time-averaged distributions of solid holdup, as depicted in Figure 5.3. Upon conducting the analysis, it was observed that the results obtained with grid resolutions of 5 by 5 mm and 7 by 7 mm were similar. Therefore, for the subsequent phases of the study, a grid resolution of 5 by 5 mm was chosen. This decision was made based on the consideration that using a 5mm grid provided comparable results while demanding less time and cost, making it a more efficient choice for the continuation of the research.

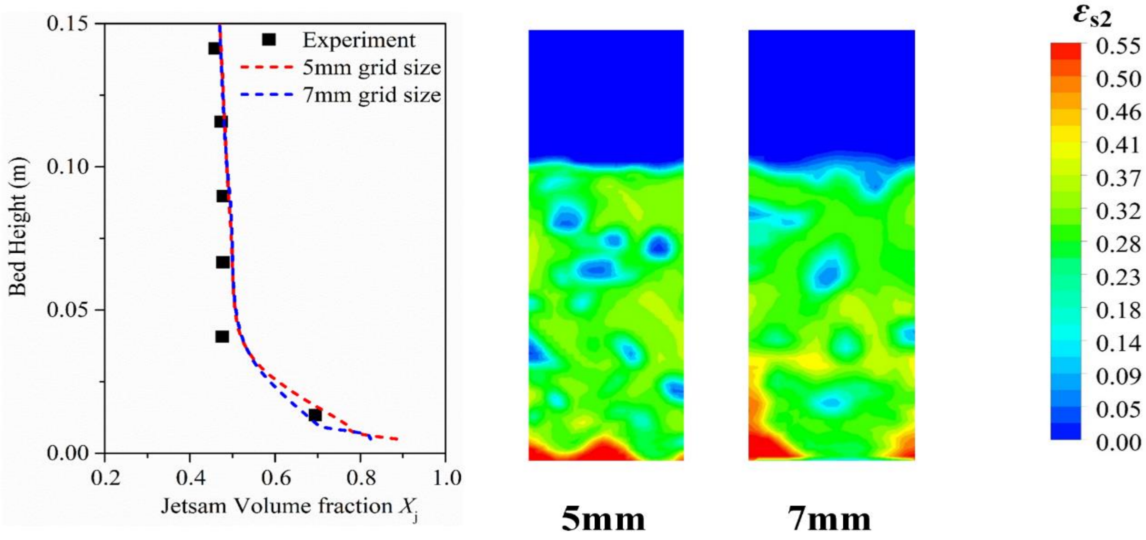

Figure 5.3: Grid Independence Test – 5mm & 7mm with Axial Profiles for Marzocchella et al [47]

5.4. Simulation Time Step Selection

In the selection of time step for the computation cost is of utmost importance, remaining factor also include the simulation complexity, overall simulation results. In this study, three time steps were analyzed 0.0002s, 0.0005s and 0.001s and found out that 0.0005s should be used, as this will be gives best results with less time. Fig 5.4 shows the comparison of results between all time steps analyzed.

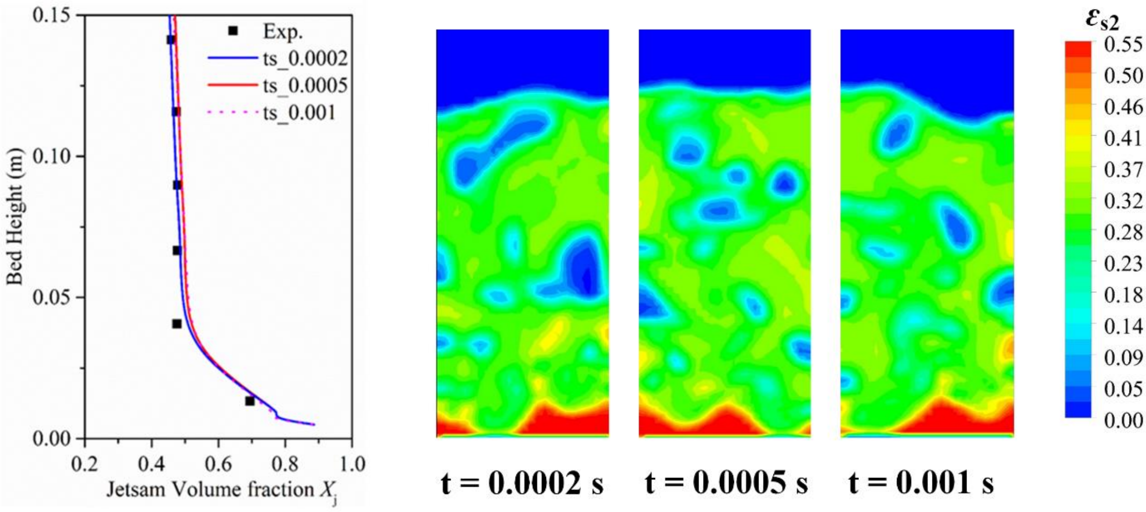

Figure 5.4: Time Selection Test for Marzocchella et al [47]

5.5. Voidage Distribution

Figure 5.5 shows the voidage distribution against different drag model applied at 1.0 sec, all drag models show similar results for voidage distribution but we have selected Gidaspow as this drag aligns with other factors very well.

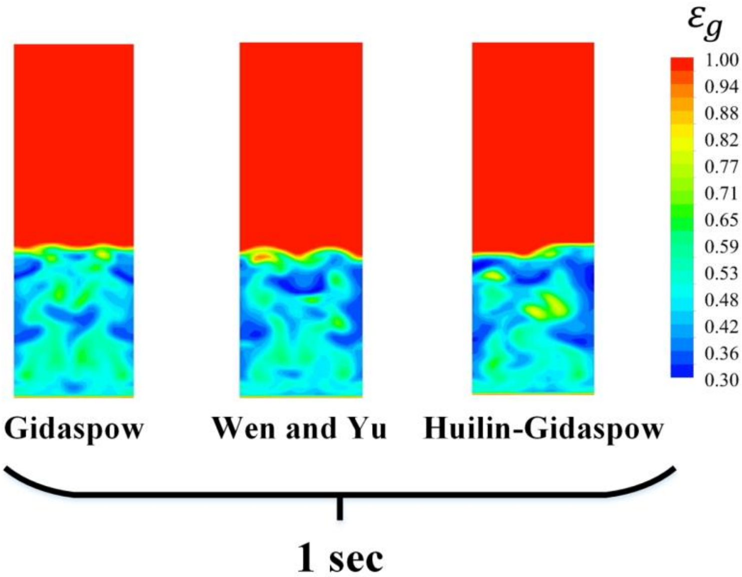

Figure 5.5: Instantaneous Voidage Distribution for Marzocchella et al [47]

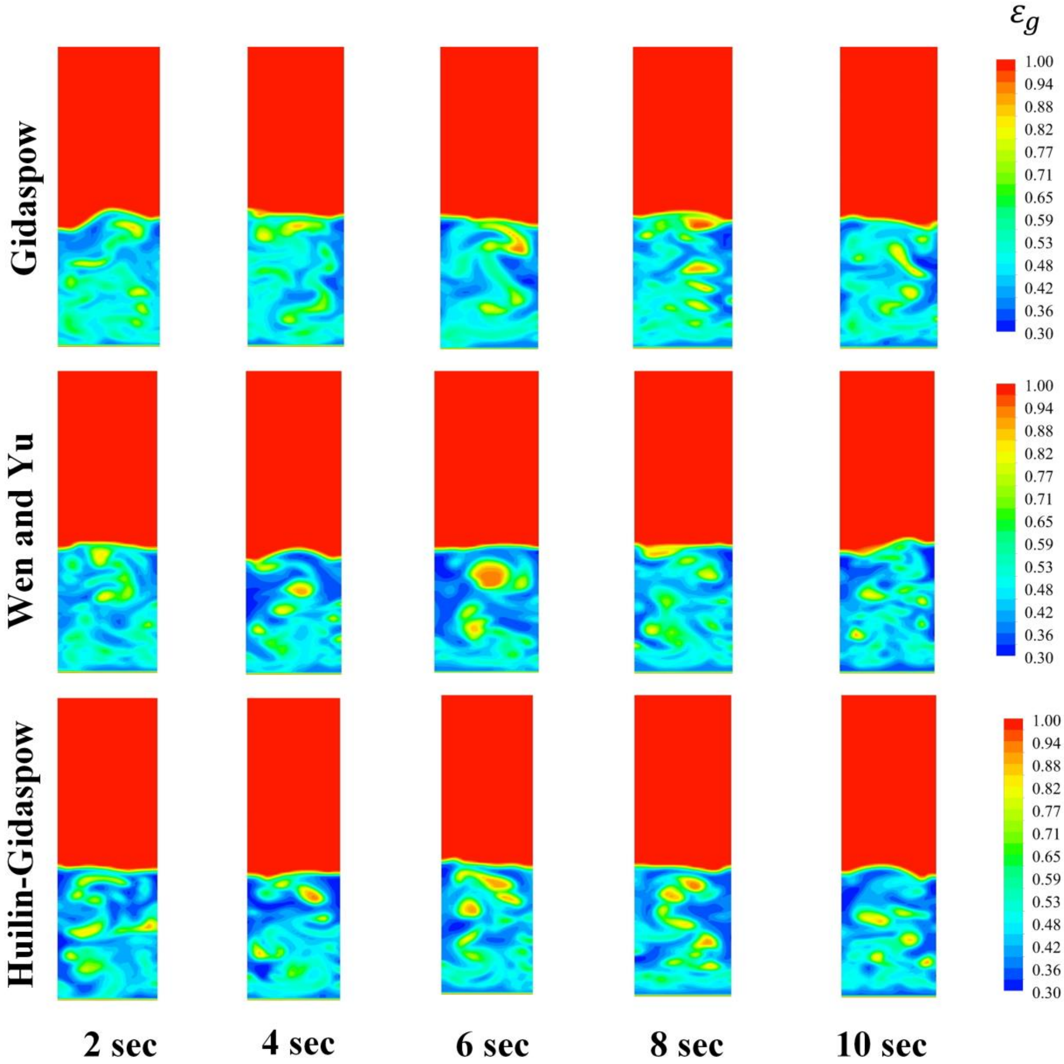

Figure 5.6: Voidage Distribution at Different Time steps for Marzocchella et al [47]

5.6. Solid Velocity

In Figure 5.7, the flotsam and jetsam particles are shown, with their colors indicating velocity magnitude. The gidaspow drag shows the velocity in the range of 0.67 m/s which is realistic then other drag models, that is why gidaspow drag was selected.

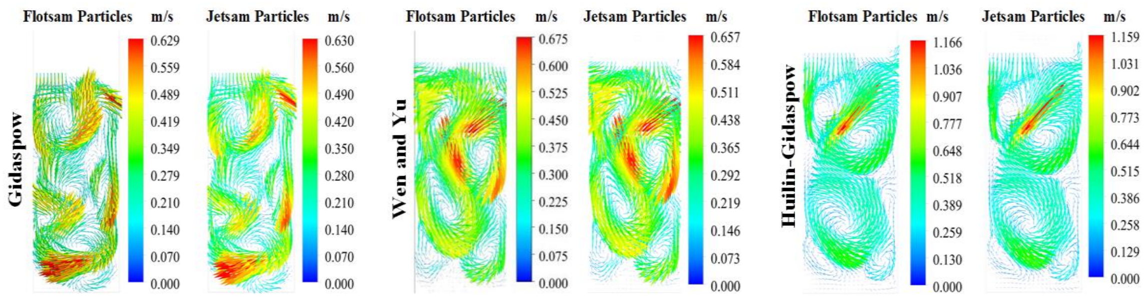

Figure 5.7: Flotsam and Jetsam Velocity Contours for Marzocchella et al [47] Using Different Drags

5.7. Solid Segregation

Figure 5. shows the contour of flotsam volume fraction utilizing various drag models discussed above.

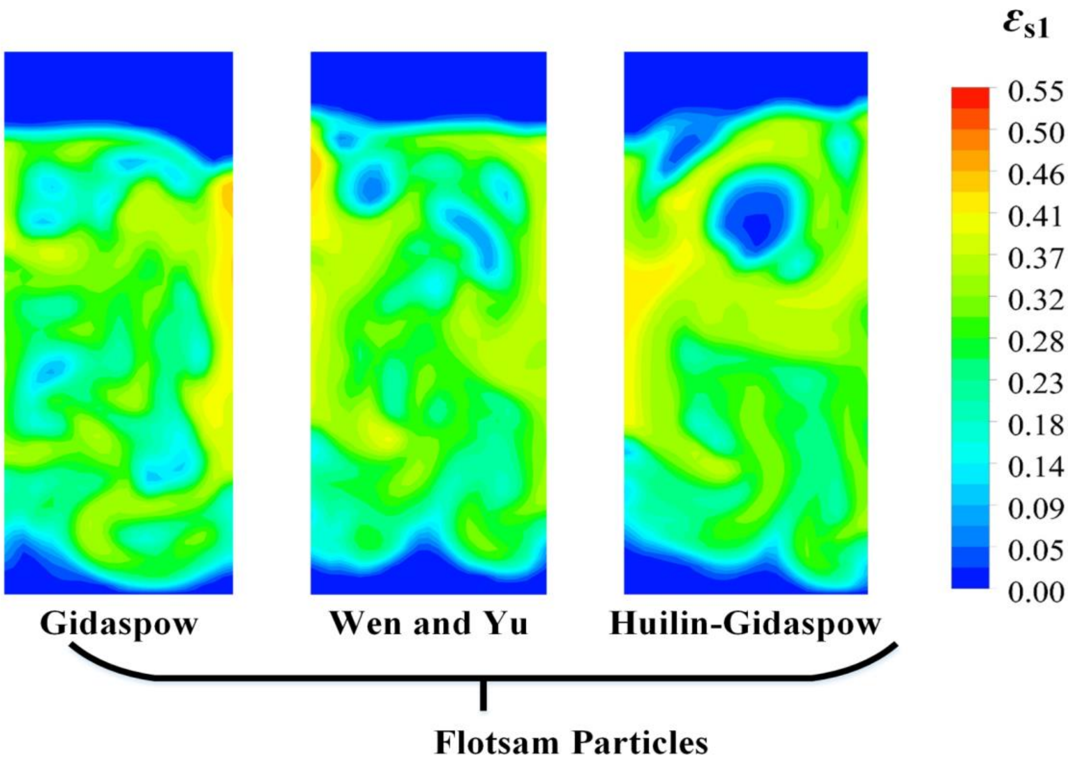

Figure 5.8: Solid Segregation Profiles Marzocchella et al [47] Using Different Drags

5.8. Axial Profiles

Figure 5.9 presents the axial profiles of Xj (where Xj represents the volume of jetsam divided by the volume of all particles) utilizing various drag models. Overall, both simulations demonstrate reasonable consistency with experimental data. However, the

Gidaspow drag model offers superior representation of the dense bottom portion of the bed compared to alternative drag models.

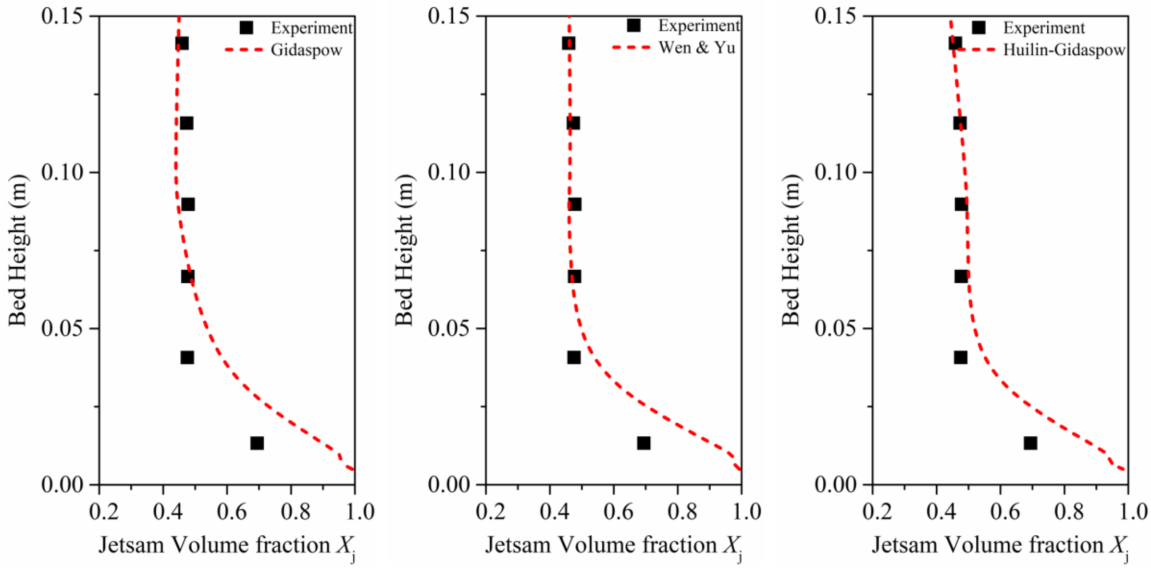

Figure 5.9: Axial Profiles of Volume Ratio of Jetsam Particles for Marzocchella et al [47] Using Different Drags

5.9. Specularity Coefficient

The specularity coefficient is an input parameter which is aimed at incorporating particle-wall collision effects. In this study, we explored several values within the range of 0 to 1 to identify the most suitable value for numerical simulations for our selected cases. The result of different value of coefficient is summarized in Figure 5.10.

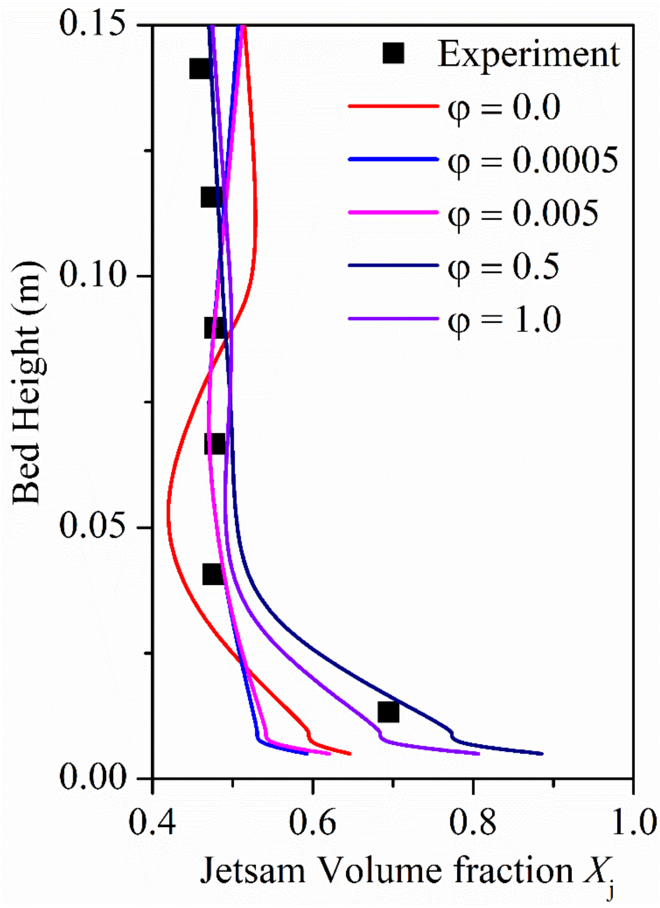

Figure 5.10: Specularity Coefficient

CHAPTER 06: CONCLUSIONS AND FUTURE RECOMMENDATIONS

In conclusion, this study addresses the formidable challenge of predicting hydrodynamics in fluidized bed reactors, specifically focusing on bubbling beds with Geldart B particles— an underexplored domain in the existing literature. Our investigation comprehensively examined the impact of various parameters, including height, width, velocity, particle diameter, initial height, solid fraction, particle density, drag scaling factor, restitution coefficient, specularity coefficient, and mesh size. This comprehensive approach contributes valuable insights and tools, paving the way for a deeper understanding and more accurate prediction of the complex dynamics within fluidized bed systems.

Based on the comprehensive exploration conducted in this study, several future recommendations emerge for further advancing the understanding and prediction of hydrodynamics in fluidized bed reactors, particularly those involving fine Geldart B particles:

1. **Parameter Sensitivity Analysis:** Conduct a detailed sensitivity analysis to identify the most influential parameters affecting solid volume fraction. Understanding the relative impact of each parameter can guide future experiments and simulations.

2. **Incorporating Additional Parameters:** Consider expanding the parameter set to encompass other potentially influential factors that were not part of the current study. Exploring a broader range of conditions can provide a more holistic view of fluidized bed dynamics.

3. **Dynamic Modeling:** Extend the modeling approach to dynamic scenarios, where the parameters evolve over time. Dynamic modeling can capture transient behaviors and provide insights into the system's response under changing conditions.

4. **Experimental Validation:** Validate the predictive capabilities of the developed models through experimental studies. Real-world data can provide valuable

validation, ensuring the reliability and applicability of the models in practical fluidized bed reactor scenarios.

5. **Interparticle Forces Investigation:** Dive deeper into the intricacies of interparticle forces, exploring different methodologies to model and quantify these forces accurately. This can involve experimental studies focused explicitly on interparticle interactions.

6. **Collaboration and Knowledge Sharing:** Foster collaboration and knowledge sharing within the scientific community working on fluidized bed reactors. Collaborative efforts can lead to the development of standardized models and benchmarks for comparison.

7. **Environmental Considerations:** Integrate environmental considerations into the modeling framework, considering factors such as emissions, energy consumption, and environmental impact. This broader perspective aligns with sustainability goals in reactor design and operation.

8. **Educational Outreach:** Develop educational resources or workshops to share the knowledge gained from this study with the wider community. This can contribute to the professional development of researchers and engineers involved in fluidized bed reactor studies.

By addressing these future recommendations, the field can advance towards more accurate predictions, improved understanding, and practical applications of fluidized bed reactor hydrodynamics, especially in the context of fine Geldart B particles.

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