Numerical Modeling and Prediction of Bubbling Fluidized Beds

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ABSTRACT

Numerical modeling and prediction techniques are used to determine pressure drop, minimum fluidization velocity and segregation for bubbling fluidized beds. The computational fluid dynamics (CFD) code Multiphase Flow with Interphase eXchange (MFIX) is used to study a two-stage reactor geometry with a binary mixture. MFIX is demonstrated to accurately predict pressure drop versus inlet gas velocity for binary mixtures. A new method is developed to predict the pressure drop versus inlet gas velocity and minimum fluidization velocity for multi-component fluidized beds. The mass accounting in the stationary system (MASS) method accounts for the changing bed composition during the fluidization process by using a novel definition for the mass fractions of the bed not yet fluidized. Published experimental data for pressure drop from single-, binary- and ternary-component fluidized bed systems are compared to MFIX simulations and the MASS method, with good agreement between all three approaches. Minimum fluidization velocities predicted using correlations in the literature were compared with the experimental data, MFIX, and the MASS method. The predicted minimum fluidization velocity from the MASS method provided very good results with an average relative error of ±4%. The MASS method is shown to accurately predict when complex multi-component systems of granular material will fluidize. The MASS method and MFIX are also used to explore the occurrence and extent of segregation in multi-component systems. The MASS method and MFIX are both shown to accurately predict the occurrence and extent of segregation in multi-component systems.
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Nomenclature

\( A \) reactor cross sectional area [cm\(^2\)]
\( \text{Ar} \) Archimedes number [-]
\( C \) randomly fluctuating velocity [cm/s]
\( c \) coefficient of friction, and instantaneous particle velocity [cm/s]
\( C_D \) drag coefficient [-]
\( C_1, C_2 \) Constants in Eq. (7)
\( D \) diameter [cm]
\( \overline{D} \) strain rate tensor [s\(^{-1}\)]
\( d_{wf} \) down-wind factor
\( e \) coefficient of restitution [-]
\( g \) gravitational acceleration [cm/s\(^2\)]
\( g_0 \) radial distribution function [-]
\( H \) reactor height [cm]
\( h \) height [cm]
\( h_0 \) initial bed height [cm]
\( I \) interactive force [N/m\(^3\)]
\( m \) mass [g]
\( n \) total number of components [-]
\( Q \) volumetric flow rate [cm\(^3\)/s]
\( q_\Theta \) diffusive flux of granular energy [J/m\(^2\) s]
\( R \) universal gas constant [Pa m\(^3\)/kmol K]
\( \text{Re} \) Reynolds number [-]
\( R_\Phi \) source term [-]
\( \overline{S} \) stress tensor [dyne/cm\(^2\)]
\( U \) inlet gas velocity [cm/s]
\( u \) velocity vector [cm/s]
\( \varphi \) volume [cm\(^3\)]
\( X \) mass fraction [-] and horizontal location [cm]
\( Z \) vertical height [cm]

Greek Letters

\( \beta \) coefficient of interphase force [g/cm\(^3\) s]
\( \Gamma_\Phi \) diffusion coefficient
\( \gamma_\Theta \) rate of granular energy dissipation [J/m\(^3\) s]
\( \Delta P \) pressure drop [Pa]
\( \varepsilon \) volume fraction [-]
\( \Theta \) granular temperature [cm\(^2\)/s\(^2\)]
\( \lambda_\text{si} \) second coefficient of viscosity [g/cm s]
\( \mu_\text{si} \) shear viscosity [g/m s]
\( \mu \) viscosity [g/cm s]
\( \xi_e \) convection weighting factor [-]
\( \rho \) density [g/cm\(^3\)]
\( \tau \) viscous stress tensor [Pa]
\( \Phi \) scalar variable [-]
\( \varphi \) blending function [-]
\( \psi \) sphericity [-]

**Subscripts**

- \( b \) bulk
- \( f \) flotsam
- \( g \) gas phase
- \( i \) individual component
- \( j \) interactive component
- \( M \) mixture
- \( mf \) minimum fluidization
- \( p \) jetsam
- \( s \) solid phase
- \( T \) total

**Superscripts**

- \( k \) discrete inlet gas velocity
- \( P \) plastic regime
- \( V \) viscous regime
Chapter 1 Introduction

1.1 Motivation

Fluidized beds have many industrial applications including combustion, gasification and chemical processing [1-6]. Fluidized bed combustion has many advantages over conventional combustion techniques including a more stable combustion environment, lower temperature combustion, more complete burnout, less fuel processing and lower pollutant production [4, 7]. Fluidized beds can also be used for the gasification and pyrolysis of solid fuels such as coal and biomass [1, 3, 8]. By converting solid fuels into gas or liquid fuels, the disadvantages of solid fuel transport, storage and pre-combustion processing can be avoided [9]. Other industrial applications also take advantage of the high heat transfer rates, stable conditions and long contact time between gas and solid phases in the formation of chemical products [3-5, 8, 10].

Demand for renewable energy sources has sparked interest in biomass combustion, pyrolysis, and gasification [11]. Unfortunately, most forms of biomass do not lend themselves to conventional combustion techniques. Biomass often has a low heating value, is irregularly shaped, moist, and difficult to process [7]. To overcome the difficulties associated with biomass combustion, pyrolysis, and gasification, fluidized bed technology is utilized [11].

Fluidized bed technology supports and stabilizes the combustion, pyrolysis and gasification of a broad range of particles, including biomass [1, 3, 7, 8, 11]. Fluidized beds are often assumed to be simple mixtures for design purposes. However, realistic fluidized beds are often complex multi-component mixtures with various particle sizes, shapes and densities. Currently, little is known about the fluidization of multi-component mixtures.
Knowledge of bed pressure drop, minimum fluidization velocity and segregation are vital to the operation, design and optimization of fluidized beds. To study fluidization and design fluidized bed reactors, experimental techniques are commonly employed on small-scale fluidized beds. It is impractical and cost prohibitive to employ such experimental techniques on large-scale fluidized beds. An alternative design technique is computational fluid dynamics (CFD) modeling of fluidized beds. CFD models can be validated using small-scale experimental reactors or industrial full-scale reactors. Validated CFD models can be used to design reactors without large pilot-scale facilities. CFD modeling of fluidized bed reactors is a challenging and growing research area due to the complexities of gas-solid interactions, solid-solid interactions, and chemical kinetics.

1.2 Objectives

This work focuses on three objectives. The first objective is the modeling and optimization of a two-stage fluidized bed reactor in the government-developed CFD code Multiphase Flow with Interphase eXchange (MFIX). The National Energy Technology Laboratory (NETL) developed MFIX to model fluid-solid flows and is an ideal code for the modeling of fluidized bed reactors. To validate the MFIX models, simulations will be compared to experimental data and a grid independence study will be performed. The validated MFIX models will then be used to optimize the two-stage reactor.

The second objective is to better understand the fluidization process for multi-component mixtures. A new method will be developed to predict the pressure drop versus inlet gas velocity and minimum fluidization velocity for multi-component fluidized beds. Published experimental data for pressure drop from single-, binary- and ternary-component fluidized bed systems will be compared to MFIX simulations and the new mass accounting in the stationary system (MASS)
method. Minimum fluidization velocities predicted using correlations in the literature will be compared with the published experimental data, MFIX, and the MASS method. Recommendations will also be made for more robust correlations.

The third objective is to better understand and predict segregation in fluidized beds. The MASS method will be used to predict the potential for segregation in multi-component mixtures and compared to MFIX simulations. The MASS method will also be used to predict average particle mass distributions throughout the reactor during the fluidization process and compared to published experimental data.

The goal of these objectives is to strengthen and advance current knowledge on multi-component fluidization. It is hoped that the MASS method and MFIX models presented here will advance the modeling, design and optimization of fluidized bed reactors in all applications.

1.3 Outline of the Thesis

Chapter 2 begins with a brief discussion on pressure drop, minimum fluidization velocity, granular beds and the operation regimes of fluidized beds. A detailed review of the various single-component and multi-component correlations currently available for predicting fluidized bed minimum fluidization velocity is then presented. Concluding Chapter 2 is a discussion on fluidized bed pyrolysis and bed segregation.

Chapter 3 presents the numerical formulations used in MFIX, which is used throughout this work to model fluidized bed reactors. The governing equations, discretization, boundary conditions and initial conditions used in MFIX are discussed in Chapter 3.

Chapter 4 outlines the modeling, validation and optimization of a two-stage reactor geometry and a binary mixture in MFIX. MFIX simulations are verified by comparing them to experimental pressure drop data and a grid resolution study is performed. The optimum
operation conditions to promote segregation within the binary mixture are then determined by performing a parametric study on inlet gas velocity.

Chapter 5 presents the theory, formulation, validation and significance of the MASS method for predicting the pressure drop versus inlet gas velocity and minimum fluidization velocity for multi-component fluidized beds. Recommendations are also made for more robust correlations.

Chapter 6 discusses the MASS methods ability to predict segregation for multi-component systems. The MASS methods ability to predict average particle distributions throughout the bed and fluidized region are also discussed.

Chapter 7 summarizes the conclusions and findings from the research presented in this Thesis. Possible future work is also suggested, which may result from the current findings.
Chapter 2 Literature Review

2.1 Fluidized Bed Terminology

Fluidized beds have a wide range of applications and therefore come in many sizes and shapes. In general, fluidized beds are cylindrical configurations with an internal reactor diameter, \( D \), height, \( H \), and cross sectional area \( A \). Figure 2.1 is a 2D schematic of a typical reactor geometry. At the base of the reactor is a distributor plate, which is typically a heavily perforated plate designed to evenly distribute the gas flow entering the bottom of the reactor. Beneath the distributor plate is a plenum region, which is designed to produce homogeneous gas temperatures and pressures. Fluidized beds operate by flowing gas upward through a bed of granular material as shown in Figure 2.1. The superficial gas velocity, \( U_g \), can be found by balancing the volumetric flow rate entering the plenum, \( Q \), with the volumetric flow rate entering the reactor chamber after passing through the distributor plate. The distributor plate is assumed to produce a uniform velocity profile, \( U_g \), across the entire reactor cross sectional area. Therefore, the superficial or inlet gas velocity can be expressed as:

\[
U_g = \frac{Q}{A}
\]  

The distributor plate and plenum regions of the domain are not typically modeled and the superficial inlet gas velocity is used as the inlet condition to the domain. Above the bed of granular material is the freeboard, which is considered to contain only gas phase. The outlet of the reactor is located above the freeboard and typically exits to atmospheric pressure.
As inlet gas velocity increases through an initially packed bed, the drag force produced by the gas on the granular material increases. The increased drag force increases pressure drop, $\Delta P$, through the bed. Eventually the drag force on the granular material equals the bed material weight and the bed completely fluidizes. Once fluidized, the pressure drop, $\Delta P_T$, across the bed remains constant with increasing gas velocity, $U_g$. The velocity at the inception of fluidization is referred to as the minimum fluidization velocity, $U_{mf}$ [12]. Knowledge about bed pressure drop and minimum fluidization velocity are useful tools in the design and operation of fluidized beds, and are commonly presented on a pressure drop curve as shown in Figure 2.2.

![Figure 2.1 Schematic of typical reactor geometry.](image)

![Figure 2.2 Relationship between pressure drop and gas inlet velocity.](image)
To help characterize particles fluidization behavior, Geldart [14] created four particle classifications or “Geldart Groups”. Geldart A particles have small diameters (20 - 100 μm), low densities (< 1.4 g/cm³), are easily fluidized, expand significantly and are representative of most granular catalysts. Geldart B particles typically have larger diameters (40 - 500 μm), medium densities (1.4 - 4.5 g/cm³), are easily fluidize, readily form bubbles and are representative of sand-like granular materials. Geldart C particles typically have very small diameters (20 - 30 μm) and are difficult to fluidize due to large cohesive forces produced within the bed. Geldart D particles typically have very large diameters (> 600 μm), and are representative of the spouting granular materials. The fluidization behavior of a system is influenced by the number of components that represent the granular material.

Fluidized beds can be described as a system consisting of granular material. Systems can be divided into chemically similar granular materials called solid phases, which can be described by particle properties such as density and diameter. Solid phases can be further divided into narrow ranges of particle properties called components, and can be modeled using a single set of characteristic properties. Characteristic-component properties are often mass-weighted or volume-weighted particle properties [13]. A bed defined by a single solid phase and a single component is a single-component system.

A bed defined of any number of solid phases and more than one component is a multi-component system. An example multi-component system is shown in Figure 2.3 for a granular mixture of two solid phases, sand and biomass, and three components distinguished by characteristic particle diameters. The fluidization behavior of a single-component system is a linear increasing relationship between pressure drop and inlet gas velocity until fluidization at \( U_{mf} \), as shown in Figure 2.4a [15]. The fluidization behavior of a multi-component system is a
nonlinear relationship as pressure drop increases until the bed is completely fluidized, as shown in Figure 2.4b [15]. Currently, estimating the minimum fluidization velocity in multi-component systems can be difficult. Many available correlations have proven unreliable at predicting the most simple of multi-component systems and provide no insight into the physics of the fluidization process [1].

![Diagram of divisions within a multi-component bed.](image)

**Figure 2.3** Example of divisions within a multi-component bed.

![Graphs showing pressure drop versus inlet gas velocity.](image)

**Figure 2.4** Typical curve for pressure drop versus inlet gas velocity for (a) single-component system and (b) multi-component system.
There are several types of fluidizing beds including bubbling and circulating. Bubbling fluidized beds (BFBs) occur when the inlet gas velocity is sufficiently above the minimum fluidization velocity to cause the formation of bubble-like structures within the granular bed material [12]. Bubbles help to promote mixing of the bed material and increase some of the benefits associated with fluidized bed technology. Circulating fluidized beds (CFBs) occur at even higher inlet velocities than BFBs and cause the bed material to entrain in the gas flow. The entrained particles are then carried out of the bed and circulated by mechanical capture back into the bed. CFBs provide significant amounts of contact time between the gas and particle material enhancing heat transfer and chemical reactions between gas and solid phases.

2.2 Single-Component System Fluidization Correlations

Relationships have been developed to predict fluidization characteristics for a single-component bed, such as pressure drop through the bed and minimum fluidization velocity. Pressure drop, $\Delta P_T$, is derived from a force balance for a bed of particles assuming negligible cohesive forces [17]:

$$\Delta P_T = \frac{mg}{A}$$  \hspace{1cm} (2)

for a bed material of mass $m$, reactor cross sectional area, $A$, and gravity $g$. Assuming gas density to be negligible in comparison to solids density it is possible to express pressure drop as:

$$\Delta P_T = \rho_b g h_0$$  \hspace{1cm} (3)

where the initial bed height is $h_0$ and the bulk density is $\rho_b = m / \mathcal{V}_0$ for an initial bed volume, $\mathcal{V}_0$. Bulk density can also be related to the solids volume fraction, $\varepsilon_s$, and solids density, $\rho_s$:

$$\rho_b = \varepsilon_s \rho_s$$  \hspace{1cm} (4)
Substituting equation (4) into equation (3) results in an alternative relationship for pressure drop [8, 10]:

$$\Delta P_T = \varepsilon_s \rho_s g h_0$$ \hspace{1cm} (5)

The established Ergun correlation is often used to predict minimum fluidization velocity, $U_{mf}$, for a single-component system. The original Ergun correlation [16] is:

$$\frac{1.75}{\psi_s \varepsilon_{mf,g}^3} \text{Re}_{mf}^2 + \frac{150 \left(1 - \varepsilon_{mf,g} \right)}{\psi_s^2 \varepsilon_{mf,g}^3} \text{Re}_{mf} = \text{Ar}$$ \hspace{1cm} (6)

where $\varepsilon_{mf,g}$ is the void fraction at fluidization and $\psi_s$ is the solids sphericity. The particle Reynolds number at fluidization is $\text{Re}_{mf} = \rho_g D_s U_{mf} / \mu_g$ and the Archimedes number is $\text{Ar} = \rho_g D_s^3 (\rho_s - \rho_g) g / \mu_g^2$ where $\rho_g$ is the gas density, $D_s$ is the solids diameter and $\mu_g$ is the gas viscosity. A simplification of equation (6) has been presented in the literature [17] by assuming that at the momentum of fluidization, the buoyancy force acting on a particle equals the drag force. Combined with the Ergun definition of the drag coefficient results in an equation for the minimum fluidization velocity [17]:

$$U_{mf} = \frac{(D_s \psi_s)^3 (\rho_s - \rho_g) g \varepsilon_{mf,g}^3}{150 \mu_g \left(1 - \varepsilon_{mf,g} \right)} \quad \text{Re}_{mf} < 20$$ \hspace{1cm} (7)

Many single-component correlations are based on simplifications of the Ergun equation at the point of fluidization. A simplification is the Wen & Yu equation [18], which removes the values of sphericity, $\psi_s$, and minimum fluidization void fraction, $\varepsilon_{mf,g}$, from the calculation, and is useful because these values are not always known for a system. The Wen & Yu correlation is:

$$\text{Re}_{mf} = \sqrt{C_1^2 + C_2 \text{Ar} - C_1}$$ \hspace{1cm} (8)

Many values have been suggested for the constants $C_1$ and $C_2$, as summarized in Table 2.1.
Table 2.1 Experimentally determined constants for use with the Wen & Yu [18] equation.

\[ \text{Re}_{mf} = \sqrt{C_1^2 + C_2 \text{Ar} - C_1} \]

<table>
<thead>
<tr>
<th>Investigator</th>
<th>( C_1 )</th>
<th>( C_2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Babu, Shah &amp; Talwalkar [19]</td>
<td>25.25</td>
<td>0.0651</td>
</tr>
<tr>
<td>Bourgeois &amp; Grenier [20]</td>
<td>25.46</td>
<td>0.03824</td>
</tr>
<tr>
<td>Chitester [21]</td>
<td>28.7</td>
<td>0.0494</td>
</tr>
<tr>
<td>Grace [22]</td>
<td>27.2</td>
<td>0.0408</td>
</tr>
<tr>
<td>Richardson &amp; St. Jeromin [23]</td>
<td>25.7</td>
<td>0.0365</td>
</tr>
<tr>
<td>Saxena &amp; Vogel [24]</td>
<td>25.28</td>
<td>0.0571</td>
</tr>
<tr>
<td>Thonglimp [25]</td>
<td>31.6</td>
<td>0.0425</td>
</tr>
<tr>
<td>Wen &amp; Yu [18]</td>
<td>33.7</td>
<td>0.0408</td>
</tr>
<tr>
<td>Zhiping [26]</td>
<td>22.1</td>
<td>0.0354</td>
</tr>
</tbody>
</table>

The Wen & Yu equation is popular because of its simplicity, however the justification for such a correlation is rather poor [27]. The lack of agreement for the experimentally determined constants \( C_1 \) and \( C_2 \) also brings into question the capability of such a model to predict the behavior of any unique system.

Other established single-component correlations are presented in Table 2.2. The Ergun correlation [16] is the only correlation presented in Table 2.2 that includes minimum fluidization void fraction, \( \varepsilon_{mf,g} \), and particle sphericity, \( \psi_s \). In an attempt to create a more simple correlation other investigators removed the dependence on \( \varepsilon_{mf,g} \) and \( \psi_s \) (see Table 2.2). Unfortunately, void fraction and particle sphericity are essential in describing the initial condition of the system, thus removing these terms will result in inaccurate predictions for minimum fluidization velocity [27].

All single-component fluidization correlations require the use of characteristic particle properties to represent the entire system. In their current form, single-component correlations are incapable of predicting the behavior of binary or multi-component systems. The following section describes how these single-component correlations can be used to model multi-component systems as well as develop multi-component relationships.
Table 2.2 Single-component minimum fluidization velocity correlations.

<table>
<thead>
<tr>
<th>Investigator</th>
<th>Correlation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Baeyens &amp; Geldart [28]</td>
<td>( \text{Ar} = 1823 \text{Re}<em>{\text{mf}}^{1.07} + 21.27 \text{Re}</em>{\text{mf}}^{2} )</td>
</tr>
<tr>
<td></td>
<td>( U_{\text{mf}} = \frac{9.125 \times 10^{-4} \left( \frac{\rho_s - \rho_g}{\rho_g} \right)^{0.934} \text{g}^{0.934} \text{D}_{s}^{1.8}}{\mu^{0.87} \rho_g^{0.066}} )</td>
</tr>
<tr>
<td>Bena [29]</td>
<td>( \text{Re}_{\text{mf}} = \frac{1.38 \times 10^{-3} \text{Ar}}{(\text{Ar} + 19)^{0.11}} )</td>
</tr>
<tr>
<td>Broadhurst &amp; Becker [30]</td>
<td>( \text{Re}_{\text{mf}} = \sqrt{\text{Ar} \left( 2.42 \times 10^5 \text{Ar}^{-0.85} \left( \frac{\rho_s}{\rho_g} \right)^{0.13} + 37.7 \right)}^{-1} )</td>
</tr>
<tr>
<td>Davies &amp; Richardson [31]</td>
<td>( \text{Re}_{\text{mf}} = 7.8 \times 10^{-4} \text{Ar} )</td>
</tr>
<tr>
<td>Doichev &amp; Akhmakov [32]</td>
<td>( \text{Re}_{\text{mf}} = 1.08 \times 10^{-3} \text{Ar}^{0.947} )</td>
</tr>
<tr>
<td>Ergun [16]</td>
<td>( \text{Ar} = \frac{1.75}{\psi^{3/2} \epsilon_{\text{mf, g}}} \text{Re}<em>{\text{mf}}^2 + \frac{150 (1 - \epsilon</em>{\text{mf, g}})}{\psi^{2/3} \epsilon_{\text{mf, g}}} \text{Re}_{\text{mf}} )</td>
</tr>
<tr>
<td>Frantz [33]</td>
<td>( \text{Re}_{\text{mf}} = 1.065 \times 10^{-3} \text{Ar} ), ( \text{Re} &lt; 32 )</td>
</tr>
<tr>
<td>Goroshko, Rozembaum &amp; Todes [34]</td>
<td>( \text{Re}_{\text{mf}} = \frac{\text{Ar}}{1400 + 5.2 \sqrt{\text{Ar}}} )</td>
</tr>
<tr>
<td>Leva [35]</td>
<td>( U_{\text{mf}} = \frac{7.169 \times 10^{-4} \text{D}_{s}^{1.82} \left( \frac{\rho_s - \rho_g}{\rho_g} \right)^{0.94} \text{g}}{\mu^{0.06} \rho_g^{0.88}} )</td>
</tr>
<tr>
<td>Miller &amp; Logwinuk [36]</td>
<td>( U_{\text{mf}} = \frac{0.00125 \text{D}_{s}^{2} \left( \frac{\rho_s - \rho_g}{\rho_g} \right)^{0.9} \rho_g^{0.1} \text{g}}{\mu} )</td>
</tr>
<tr>
<td>Pillai &amp; Raja Rao [37]</td>
<td>( U_{\text{mf}} = \frac{7.01 \times 10^{-4} \text{D}_{s}^{2} \left( \frac{\rho_s - \rho_g}{\rho_g} \right) \text{g}}{\mu} )</td>
</tr>
<tr>
<td>Riba, Routie &amp; Couderc [38]</td>
<td>( \text{Re}_{\text{mf}} = 1.54 \times 10^{-2} (Ga)^{0.66} M\nu^{0.7} ), ( 10 &lt; \text{Re} &lt; 1000 )</td>
</tr>
<tr>
<td></td>
<td>( Ga = D_{s}^{3} \rho_g^{2} \text{g} / \mu \text{g}^2 )</td>
</tr>
<tr>
<td></td>
<td>( M\nu = \left( \rho_s - \rho_g \right) / \rho_g )</td>
</tr>
<tr>
<td>Wen &amp; Yu [18]</td>
<td>( \text{Re}_{\text{mf}} = \sqrt{C_1^2 + C_2 \text{Ar} - C_1} )</td>
</tr>
</tbody>
</table>
2.3 Multi-Component System Fluidization Correlations

Many approaches have been suggested to define multi-component systems. In general, three approaches that have been applied to predict the minimum fluidization velocity are: (1) mass-weighted mixture properties, (2) mass-weighted mixture dimensionless numbers and (3) system-specific correlations.

2.3.1 Mass-Weighted Mixture Properties

The first approach involves treating the multi-component system as a single-component system by determining mixture properties, such as a mixture density or mixture diameter. By implementing mixture properties for a multi-component system, it is possible to use the single-component equations to determine the minimum fluidization velocity of the mixture. The most common technique for determining mixture properties uses weighted averages of the multi-component system. These weighted averages can be based on volume fractions, but are more commonly expressed as mass fractions. The mass fraction, $X_i$, of an individual component $i$ is:

$$X_i = \frac{m_i}{m}$$

where $m_i$ is the component mass. Some examples of weighted averages are reported by Chien-Song et al. [13] and summarized in Table 2.3, it is not obvious which method is best. Each of these methods produce different values for mixture density and mixture diameter depending on the composition. It has been suggested by Chien-Song et al. [13] that method 2 or 3 is best for determining characteristic properties.
2.3.2 Mass-Weighted Mixture Dimensionless Numbers

The second approach involves creating weighted averages of the Archimedes and Reynolds numbers. These weighted averages can then be used with single-component equations to determine the minimum fluidization velocity. Two examples of mass-weighted mixture dimensionless numbers are reported by Chien-Song et al. [13] and summarized in Table 2.4. Both methods avoid determining mixture properties and instead define mixture dimensionless numbers to describe the behavior of the entire system. There is little support for creating mixture dimensionless numbers and Chien-Song et al. [13] have shown the technique to be unreliable for capturing the true system behavior.

Table 2.3 Examples of weighted averages used to determine effective particle properties for multi-component systems [13].

<table>
<thead>
<tr>
<th>Method 1</th>
<th>Method 2</th>
<th>Method 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \rho_M = \sum (X_i \rho_i) )</td>
<td>( \rho_M = \left[ \sum (X_i / \rho_i) \right]^{-1} )</td>
<td>( \rho_M = \left[ \sum (X_i / \rho_i) \right]^{-1} )</td>
</tr>
<tr>
<td>( D_M = \left[ \sum (X_i / D_i) \right]^{-1} )</td>
<td>( D_M = \left[ \rho_M \sum (X_i / D_i / \rho_i) \right]^{-1} )</td>
<td>( D_M = \left[ \sum (X_i / D_i) \right]^{-1} )</td>
</tr>
<tr>
<td>( \text{Ar} = D_M^3 \rho_s \left( \rho_M - \rho_g \right) g / \mu^2 )</td>
<td>( \text{Ar} = D_M^3 \rho_s \left( \rho_M - \rho_g \right) g / \mu^2 )</td>
<td>( \text{Ar} = D_M^3 \rho_s \left( \rho_M - \rho_g \right) g / \mu^2 )</td>
</tr>
<tr>
<td>( \text{Re} = D_M U \rho_s / \mu )</td>
<td>( \text{Re} = D_M U \rho_s / \mu )</td>
<td>( \text{Re} = D_M U \rho_s / \mu )</td>
</tr>
</tbody>
</table>

Table 2.4 Examples of weighted averages used to determine effective non-dimensional numbers and minimum fluidization velocity for multi-component systems [13].

<table>
<thead>
<tr>
<th>Method 1</th>
<th>Method 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{Re}_i = D_i U \rho_g / \mu )</td>
<td>( \text{Re}_i = D_i U \rho_g / \mu )</td>
</tr>
<tr>
<td>( \text{Ar}_i = D_i^3 \rho_g \left( \rho_i - \rho_g \right) g / \mu^2 )</td>
<td>( \text{Ar}_i = D_i^3 \rho_g \left( \rho_i - \rho_g \right) g / \mu^2 )</td>
</tr>
<tr>
<td>( \text{Ar} = \sum (X_i \text{Ar}_i) )</td>
<td>( \text{Ar} = \left[ \sum (X_i / \text{Ar}_i) \right]^{-1} )</td>
</tr>
<tr>
<td>( \text{Re} = \sum (X_i \text{Re}_i) )</td>
<td>( \text{Re} = \sum (X_i \text{Re}_i) )</td>
</tr>
</tbody>
</table>
2.3.3 System-Specific Correlations

The development of system specific correlations is based on experimental data for a specific set of conditions, and a few examples are summarized in Table 2.5. These correlations may require information about the minimum fluidization velocity and mass fraction of each component in the system. Applying these correlations to other systems can be extremely inaccurate. One of the most notable limitations is the inability of the correlations to predict fluidization for beds comprised of more than two components. Only the correlation presented by Obata et al. [41] can be used with an unlimited number of components presuming the minimum fluidization velocity for each component is known, which is often not the case.

Table 2.5 Examples of correlations used to determine minimum fluidization velocity of multi-component systems.

<table>
<thead>
<tr>
<th>Investigator</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bilbao et al. [8]</td>
<td>$U_{mf}^m = U_{mf}^c - \left(U_{mf}^c - U_{mf}^f\right)Z_f$</td>
</tr>
<tr>
<td></td>
<td>$Z_f = \frac{X_f}{X_f + \frac{\rho_f}{\rho_p}(1 - X_f)}$</td>
</tr>
<tr>
<td>Cheung et al. [39]</td>
<td>$U_{mf} = U_s \left(U_b / U_s \right)Xb^2$</td>
</tr>
<tr>
<td>Chiba et al. [40]</td>
<td>$U_{mf} = U_f \left(\rho_m / \rho_f\right) \left(D_m / D_f\right)^2$</td>
</tr>
<tr>
<td></td>
<td>where $\rho_m = f_{mf} \rho_f + (1 - f_{mf}) \rho_p$</td>
</tr>
<tr>
<td></td>
<td>$D_m = \left[f_{nf} D_f^3 + (1 - f_{nf}) D_p^3 \right]^{1/3}$</td>
</tr>
<tr>
<td></td>
<td>$f_{nf} = \left[1 + \left(\frac{1}{X_f} - 1\right) \rho_f / \rho_p\right]^{1}$</td>
</tr>
<tr>
<td></td>
<td>$f_{mf} = \left[1 + \left(\frac{1}{X_f} - 1\right) \rho_f / \rho_p\right]^{1}$</td>
</tr>
<tr>
<td>Obata et al. [41]</td>
<td>$U_{mf} = \left[\sum X_i / U_{mf,i}\right]^{-1}$</td>
</tr>
<tr>
<td>Uchida et al. [42]</td>
<td>$U_{mf} = U_f \left(U_p / U_f \right) \left(1 - V_f\right)^m$</td>
</tr>
<tr>
<td></td>
<td>where $m = 0.17 \left[D_p / D_f \left(\rho_f / \rho_p\right)\right]^{0.437}$</td>
</tr>
<tr>
<td></td>
<td>$V_f =$ volume fraction</td>
</tr>
</tbody>
</table>
Most applications of fluidized beds are complex multi-component systems with large variations in component properties. It is important to develop models that can accurately predict fluidization characteristics for a broad range of systems. Furthermore, the existing correlations presented so far do not provide insight into the fluidization process.

2.4 Pyrolysis in Fluidized Beds

Pyrolysis is the thermal decomposition of solid fuels, such as biomass, in the absence of oxygen to form charcoal, bio-oil and fuel gas [9, 11, 63]. Pyrolysis of biomass can be performed using fluidized beds of inert material (thermal cracking), which provide excellent heat transfer and the necessary energy to vaporize volatiles. Unfortunately, pyrolysis of biomass in inert material often results in unstable fuels with low heating values and corrosive qualities that make these fuels less than ideal [64]. To remedy these issues fluidized beds are operated with active fluid catalytic cracking (FCC) materials that improve the fuel stability, heating values and corrosiveness [64]. Aspects of both thermal cracking and fluid catalytic cracking are desirable for the pyrolysis of biomass. Attempts have been made to couple thermal and catalytic cracking using a series of reactors to produce more desirable fuels [64, 65]. Another method to couple thermal and catalytic cracking is to combine the series of separate reactors into one reactor. For a single reactor to operate as two reactors the inert bed material and FCC must be maintained in separate regions of the reactor. One method to maintain separate regions within a reactor is to intentionally design the reactor so that heavy segregation takes place between the inert material and the FCC. The lower region would provide excellent heat transfer while the upper region would facilitate the formation of desirable fuels. A single reactor would require less space, less construction costs and lower operation costs while providing higher quality fuels.
2.5 Segregation in Fluidized Beds

Knowledge of bed material segregation is necessary to properly operate the two-stage reactor. Segregation in fluidized beds occurs for several reasons including size segregation, density segregation and flow regime segregation. Many studies have investigated size segregation of particles with equal density and different diameters [66, 67]. The resulting trend from these studies is that particles of large diameter segregate to the lower regions of the fluidized bed, while smaller diameter particles segregate to the upper regions. Other studies have investigated density segregation of particles with similar diameters and different densities [68]. The resulting trend found by these studies is that more dense particles segregate to the lower regions of the fluidized bed, while less dense particles segregate to the upper regions. Studies have also been performed on the role of flow regime in segregation [6]. The work of Formisani et al. [1, 2] suggested that segregation occurs up till the point of fluidization and once fully fluidized the bed becomes fully mixed exhibiting little segregation. Other studies show that the flow regime and bubble dynamics determine the extent of segregation in the fluidized bed [6, 68]. Currently little is known about predicting the extent of segregation or predicting particle distributions in fluidizing beds [69].
Chapter 3 Numerical Approach

The computational code **Multiphase Flow with Interphase eXchange** (MFIX) is described in this chapter. The basic governing equations, discretization and modeling techniques used in MFIX to represent reactors are discussed in this chapter.

3.1 Governing Equations

The numerical model used in MFIX is an Eulerian-Eulerian model. Eulerian-Eulerian models represent gas and solid components as interpenetrating continua. Each material in the model has different properties and interactions. The percent of volume occupied by a particular material over any averaging volume is given by the material volume fraction or in the case of a gas by the void fraction. The summation of the void fraction and the solid component volume fractions must equal unity:

\[ \varepsilon_g + \sum_{i=1}^{n} \varepsilon_{si} = 1 \]  

(10)

where \( \varepsilon_g \) is the void fraction or gas volume fraction, \( \varepsilon_i \) is the solid component volume fraction, \( i \) is the solid component index and \( n \) is the total number of components in the system.

3.1.1 Conservation of Mass

The continuity equations are solved for the gas phase and each solid phase to conserve mass. Assuming no generation or destruction within the phases, the continuity equations for the gas phase and solid phase, respectively, are given as:

\[ \frac{\partial}{\partial t} \left( \varepsilon_g \rho_g \right) + \nabla \cdot \left( \varepsilon_g \rho_g \mathbf{u}_g \right) = 0 \]  

(11)

\[ \frac{\partial}{\partial t} \left( \varepsilon_{si} \rho_{si} \right) + \nabla \cdot \left( \varepsilon_{si} \rho_{si} \mathbf{u}_{si} \right) = 0 \]  

(12)
where \( \mathbf{u} \) is the velocity vector, \( \rho \) is the density and the subscripts \( g \) and \( s \) represent the gas and solid phases, respectively, and subscript \( i \) represents the solid phase component.

### 3.1.2 Equation of State

The gas phase equation of state adheres to the ideal gas law:

\[
\rho_g = \frac{P_g MW}{RT_g}
\]

(13)

where \( P_g \) is the gas pressure, \( MW \) is the gas molecular weight, \( R \) is the universal gas constant and \( T_g \) is the temperature of the gas.

### 3.1.3 Conservation of Momentum

The momentum equations for gas and solid phases are, respectively:

\[
\frac{\partial}{\partial t} \left( \varepsilon_g \rho_g \mathbf{u}_g \right) + \nabla \cdot \left( \varepsilon_g \rho_g \mathbf{u}_g \mathbf{u}_g \right) = -\varepsilon_g \nabla P_g + \nabla \cdot \bar{S}_g - \sum_{i=1}^{N} I_{gi} + \varepsilon_g \rho_g g
\]

(14)

\[
\frac{\partial}{\partial t} \left( \varepsilon_i \rho_i \mathbf{u}_i \right) + \nabla \cdot \left( \varepsilon_i \rho_i \mathbf{u}_i \mathbf{u}_i \right) = -\varepsilon_i \nabla P_g + \nabla \cdot \bar{S}_{si} + I_{gi} - \sum_{j=1}^{N} I_{ij} + \varepsilon_i \rho_i g
\]

(15)

The first term on the left side is the time rate of net momentum increase and the second term is the net rate of convective momentum transfer. The right side contains a buoyancy term from the fluid pressure gradient, \( P_g \), stress tensor term, \( \bar{S} \), interaction force between solid component \( i \) and the gas phase, \( I_{gi} \), interaction force, \( I_{ij} \), between solid components \( i \) and \( j \), and gravitational forces, \( g \). The interaction forces account for momentum transfer between the gas and solid components.

### 3.1.4 Gas-Solid Interaction

The gas-solid interaction forces are the product of the coefficient of interphase force, \( \beta_{gi} \), and the slip velocity:
\[ I_{gi} = \beta_{gi} (u_g - u_{si}) \]  
\[ \beta_{gi} = (1 - \varphi_{gs}) \beta_{gi(Ergun)} + \varphi_{gs} \beta_{gi(Wen-Yu)} \]

The blending function, \( \varphi_{gs} \), is used to blend the Ergun and Wen-Yu interphase force models together. The blending function prevents discontinuities of the two models and is given as:

\[ \varphi_{gs} = \frac{\arctan \left[ 150 \times 1.75 \left( 0.2 - \left( 1 - \varepsilon_g \right) \right) \right]}{\pi} + 0.5 \]

where the drag coefficient \((C_D)\) is given as:

\[ C_D = \frac{24}{\varepsilon_g \cdot \text{Re}_{si}} \left[ 1 + 0.15 \left( \varepsilon_g \cdot \text{Re}_{si} \right)^{0.687} \right] \]

The validity of the Gidaspow drag model has been demonstrated for different materials [48-55] and is used throughout this study.

### 3.1.5 Solid-Solid Interaction

The solids-solids interaction forces are the product of the coefficient of interphase force, \( \beta_{si} \), and the slip velocity:

\[ I_{sij} = \beta_{sij} (u_{si} - u_{sj}) \]
where the subscript $i$ represents the solid component being solved in the momentum equation and the coefficient of interphase force, $\beta_{sij}$, was derived by Syamlal [45]:

$$\beta_{sij} = 3(1 + e) \left( \frac{\pi}{2} + c_{sij} \frac{\pi^2}{8} \right) \frac{(D_{si} + D_{sj})^2}{2\pi \rho_{si} \rho_{sj}} \rho_{si} \rho_{sj} g_0 |u_{sj} - u_{si}|$$ (23)

where $e$ is the coefficient of restitution, $c_{ij}$ is the coefficient of friction, and $g_0$ is the radial distribution function at contact for a mixture of spheres derived by Lebowitz [43]:

$$g_0 = \frac{1}{\varepsilon_g} + \frac{3D_{si}D_{sj}}{\varepsilon_g^2 (D_{si} + D_{sj})} \sum_{i=1}^{N} \frac{\varepsilon_{si}}{D_{si}}$$ (24)

### 3.1.6 Gas Phase Stress Tensor

The gas phase stress tensor is composed of two terms, the first is based on the pressure of the gas and the second is based on the Newtonian form of the viscous stress tensor, $\tau_g$:

$$\bar{S}_g = -P_g I + \tau_g$$ (25)

where the viscous stress tensor is:

$$\tau_g = 2\varepsilon_g \mu_g D_g + \varepsilon_g \lambda_g tr(D_g) I$$ (26)

where the strain rate tensor for the gas is:

$$\bar{D}_g = \frac{1}{2} \left[ \nabla \cdot u_g + (\nabla \cdot u_g)^T \right]$$ (27)

### 3.1.7 Solids Phase Stress Tensor

Two flow regimes are used to model the granular flow in MFIX. The plastic regime models slow shearing behavior resulting from Coulomb friction between tightly packed particles. The viscous regime models rapidly shearing behavior resulting from momentum transfers due to collisions or translations. The solids phase stress tensor is defined for both plastic and viscous regimes using the critical void fraction, $\varepsilon_g^*$, to determine the regime:
\[
\begin{align*}
S_{si} &= \begin{cases} 
-P_{si}^p I + \tau_{si} & \text{if } \varepsilon_g \leq \varepsilon_{g}^* \\
-P_{si}^v I + \tau_{si} & \text{if } \varepsilon_g > \varepsilon_{g}^*
\end{cases} 
\tag{28}
\end{align*}
\]

where the superscripts \( P \) and \( V \) represent the plastic and viscous regimes, respectively. \( P_{si} \) and \( \tau_{si} \) represent the granular pressure and viscous stress, respectively. The critical void fraction is usually equal to the void fraction at minimum fluidization, \( \varepsilon_{mf} \), for fluidized beds.

For the viscous regime the granular pressure follows the form determined by Lun et al. [56]:

\[
P_{si}^v = K_{1si} \varepsilon_{si}^2 \Theta_{si} \tag{29}
\]

where \( \Theta_{si} \) is the granular temperature and the value of \( K_{1si} \) is:

\[
K_{1si} = 2(1 + e) \rho_{si} g_0 \tag{30}
\]

The granular viscous stress is:

\[
\tau_{si} = 2 \mu_{si}^v \overline{D}_{si} + \hat{\lambda}_{si}^v \text{tr}(\overline{D}_{si}) I 
\tag{31}
\]

where \( \mu_{si}^v \) is the shear viscosity, \( \overline{D}_{si} \) is the strain rate tensor and \( \hat{\lambda}_{si}^v \) is the second coefficient of viscosity respectively defined as:

\[
\mu_{si}^v = K_{3si} \varepsilon_{si} \sqrt{\Theta_{si}} \tag{32}
\]

\[
\overline{D}_{si} = \frac{1}{2} \left[ \nabla \cdot \mathbf{u}_{si} + (\nabla \cdot \mathbf{u}_{si})^T \right] \tag{33}
\]

\[
\hat{\lambda}_{si}^v = K_{2si} \varepsilon_{si} \sqrt{\Theta_{si}} \tag{34}
\]

where the value of \( K_{2si} \) is:

\[
K_{2si} = \frac{4 D_{si} \rho_{si} (1 + e) \varepsilon_{si} g_0}{3 \sqrt[3]{\pi}} - \frac{2}{3} K_{3si} \tag{35}
\]

where the value of \( K_{3si} \) is:
For the plastic regime the granular pressure is defined as:

$$ P_{si}^p = \varepsilon_{si} P^* $$

(37)

where $P^*$ is described by an empirical power law:

$$ P^* = A(\varepsilon_g^* - \varepsilon_g)^n $$

(38)

with $A = 10^{25}$ and $n = 10$.

The solids stress tensor is calculated using the formulation of Shaeffer [57]:

$$ \tau = 2\mu_{si}^p D_{si} $$

(39)

### 3.1.8 Conservation of Granular Energy

The stress tensor of the solids phase is described by the kinetic theory of smooth, spherical particles. The granular temperature of the solids phase, $\Theta_{si}$, is related to the randomly fluctuating component of the instantaneous particle velocity, $C_{si}$:

$$ \frac{3}{2} \Theta_{si} = \frac{1}{2} \left< C_{si}^2 \right> $$

(40)

where the fluctuating component relates to the instantaneous particle velocity, $c_{si}$, by:

$$ c_{si} = u_{si} + C_{si} $$

(41)

The transport of the granular energy is:

$$ \frac{3}{2} \left[ \frac{\partial (\varepsilon_{si} \rho_{si} \Theta_{si})}{\partial t} \right. $$

$$ \left. + \nabla \cdot \left( \varepsilon_{si} \rho_{si} \Theta_{si} \mu_{si} \right) \right] = \overline{\varepsilon_{si}} : \nabla \cdot u_{si} - \nabla \cdot q_{\varepsilon_{si}} - \gamma_{\Theta_{si}} + \phi_{si} + \sum_{j=1}^{N} \phi_{ji} $$

(42)

where $q_{\varepsilon_{si}}$ is the diffusive flux of granular energy:

$$ q_{\varepsilon_{si}} = -k_{\varepsilon_{si}} \nabla \cdot \Theta_{si} $$

(43)
and $\gamma_{\theta_s}$ is the rate of granular energy dissipation due to inelastic collisions:

$$\gamma_{\theta_s} = K_{ss} \varepsilon_s^3 \Theta_s^2$$  \hspace{1cm} (44)

the remaining two terms account for the transfer of granular energy to the gas, $\Theta_{gi}$, and between the $i^{th}$ and $j^{th}$ solids, $\Theta_{ji}$. MFIX ignores the transfer between solids phases therefore $\Theta_{ji} = 0$. The transfer of granular energy between solids and the gas is given by Ding and Gidaspow [58]:

$$\phi_{gi} = -3 F_{gi} \Theta_s$$  \hspace{1cm} (45)

Further information on the numerical models used within MFIX can be found in the MFIX theory guide [46] and the MFIX summary of equations [47].

### 3.2 Numerical Formulation

To ensure the stability and accuracy of MFIX, the governing equations are discretized using a finite volume approach. An advantage of the method is that it ensures conservation of mass, momentum and energy. The finite volume method is also useful when modeling large domains where fine grids are computationally expensive and course grids must be used.

#### 3.2.1 Staggered Grid

Staggered grids avoid discretization errors produced on collocated grids such as odd-even decoupling. Odd-even decoupling occurs when odd nodes and even nodes become independent from one another and can no longer exchange information through the discretized governing equations. Odd-even decoupling results in unphysical checkerboard solutions for pressure and velocity on 2D grids. To avoid odd-even decoupling, MFIX uses a staggered grid that stores pressure, void fraction, temperature and mass fraction scalars at cell centers while velocity components are stored at cell faces. Staggered grids ensure that odd-even decoupling can not occur.
3.2.2 Discretization

The transport equation for the scalar variable \( \Phi \) is used to discuss the discretization of the governing equations:

\[
\frac{\partial}{\partial t} (\varepsilon_i \rho_i \Phi) + \frac{\partial}{\partial x_m} (\varepsilon_i \rho_i u_{im} \Phi) = \frac{\partial}{\partial x_m} \left( \Gamma_\Phi \frac{\partial \Phi}{\partial x_m} \right) + R_\Phi
\]

where \( \Gamma_\Phi \) is the diffusion coefficient for \( \Phi \) and the source term is \( R_\Phi \).

Equation (46) possesses the features of multiphase flow equations with the exception of the interphase transfer terms. The discretization of the interphase transfer terms will be discussed separately. The equation can be integrated over a control volume with nomenclature shown in Figure 3.1. The center of the cell is denoted as P and its neighboring points are referred to as E, W, N, S, T, and B with the half-node positions denoted as e, w, n, s, t, b.

Figure 3.1 Computational cell for scalar equations
A simple discretization example is a one-dimensional scalar equation. In this example the convection-diffusion terms in the x-direction are:

\[ \rho u \frac{\partial \Phi}{\partial x} - \frac{\partial}{\partial x} \left( \Gamma \frac{\partial \Phi}{\partial x} \right) \]  \hspace{1cm} (47)

Integrating equation (47) over the control volume shown in Figure 3.2:

\[ \int \left[ \rho u \frac{\partial \Phi}{\partial x} - \frac{\partial}{\partial x} \left( \Gamma \frac{\partial \Phi}{\partial x} \right) \right] dV = \left[ \rho u \Phi_e - \left( \Gamma \frac{\partial \Phi}{\partial x} \right)_e \right] A_e - \left[ \rho u \Phi_w - \left( \Gamma \frac{\partial \Phi}{\partial x} \right)_w \right] A_w \]  \hspace{1cm} (48)

Assuming piecewise-linear profiles between the grids, the second order accurate diffusive flux at the east-face is:

\[ \left( \Gamma \frac{\partial \Phi}{\partial x} \right)_e \approx \Gamma_e \frac{\Phi_e - \Phi_p}{\delta x_e} \]  \hspace{1cm} (49)

with other fluxes being similar.

To prevent numerical diffusion that may occur with first-order schemes it is common practice to employ higher-order schemes. Unfortunately, higher order schemes are not without their limitations and issues. Many higher-order schemes encounter oscillations around discontinuities. To avoid these undesirable and unrealistic oscillations, total variation diminishing (TVD) schemes are sometimes employed. A limiter is imposed on the dependent variables in TVD schemes [61]. An example of a TVD scheme is shown using \( \Phi_e \) at the east-face:
\[
\Phi_e = \xi_e \Phi_E + \bar{\xi}_e \Phi_P
\]  

(50)

where \(\xi_e\) is the convection weighting factor and \(\bar{\xi}_e = 1 - \xi_e\).

The down-wind factor, \(dwf_e\), is used to calculate the convection weighting factor:

\[
\Phi_e = \begin{cases} 
\xi_e = dwf_e & \text{if } u_e \geq 0 \\
\bar{\xi}_e = 1 - dwf_e & \text{if } u_e < 0 
\end{cases}
\]

(51)

The superbee method is utilized to determine the \(dwf_e\) and is applicable to explicit diffusion and conservation convection schemes of any order [62]:

\[
dwf_e = \frac{1}{2} \max \left[ 0, \min(1, 2\theta), \min(2, \theta) \right]
\]

(52)

where \(\theta = \Phi_C / (1 - \Phi_C)\) and the term \(\Phi_C\) is:

\[
\Phi_C = \begin{cases} 
\frac{\Phi_p - \Phi_W}{\Phi_E - \Phi_W} & \text{if } u_e \geq 0 \\
\frac{\Phi_E - \Phi_E}{\Phi_P - \Phi_E} & \text{if } u_e < 0 
\end{cases}
\]

(53)

where the locations refer to those shown in Figure 3.3. The discretized form of the transient term is:

\[
\int \frac{\partial}{\partial t} (\varepsilon, \rho, \Phi) dV \approx \left[ (\varepsilon, \rho, \Phi)_p - (\varepsilon, \rho, \Phi)_p \right] \frac{\Delta V}{\partial t}
\]

(54)

Figure 3.3 TVD scheme node locations
here the superscript 0 represents the value at the previous step in time. Source terms are typically linearized due to their nonlinear tendencies:

\[ R_\phi \approx \overline{R}_\phi - R'_\phi \Phi_p \]  \hspace{1cm} (55)

where the constant portion of \( R_\phi \) is \( \overline{R}_\phi \) and the coefficient of \( \Phi_p \) is \( R'_\phi \). The resulting source term integration is:

\[ \int R_\phi dV \approx \overline{R}_\phi \partial V - R'_\phi \Phi_p \partial V \quad \text{where} \quad R'_\phi \geq 0. \]  \hspace{1cm} (56)

The linear equation for \( \phi \) with source term \( b \) can represent all scalar equations:

\[ a_p \Phi_p = \sum_{nb} a_{nb} \Phi_{nb} + b \]  \hspace{1cm} (57)

3.3 Boundary Conditions

In fluidized beds the inlet gas passes through a distributor plate, which produces a relatively uniform inlet gas velocity profile. To model the inlet a mass inlet boundary condition is used. Only the gas phase is present in the inlet stream and enters with a uniform velocity profile and homogeneous: temperature and pressure. The outlet boundary condition is a pressure outlet. The gas phase pressure at the outlet of the reactor is equal to atmospheric. The wall boundary condition is a no slip condition for the gas phase interaction and a partial slip condition for the solids interactions. The no slip condition is shown in Figure 3.4 for a cell that encompasses the wall and states that:

\[ (U)_{\text{ghost cell}} = -(U)_{\text{near wall cell}} \]  \hspace{1cm} (58)

The partial slip condition for the solids phase follows the form determined by Hui et al. [60] and Johnson & Jackson [59]:

\[ U_{i,W} = -\frac{6\mu_i e_{\text{max}}}{\sqrt{3\pi} \rho_i c_i g_0 \sqrt{\Theta_i}} \frac{\partial U_{i,W}}{\partial n} \]  \hspace{1cm} (59)
\[ \Theta_{i,W} = -\frac{k_i \Theta_i}{\gamma_{i,W}} \frac{\partial \Theta_{i,W}}{\partial n} + \frac{\sqrt{3} \pi \phi' \rho_i \varepsilon_i U_{i,slip}^2 \varepsilon_0 \Theta^2}{6 \varepsilon_{max} \gamma_{i,W}} \]  

(60)

where \( n \) is the direction normal to the wall pointing from the fluid into the wall, \( \varepsilon_{max} \) is the maximum solids packing volume fraction (0.65), the slip velocity is \( U_{slip} = U_i - U_{i,W} \), \( \phi' \) is the specularity coefficient (0.01), \( \gamma_{i,W} \) is the collision dissipation of granular temperature, and \( U_{i,W} \) is the solids velocity at the wall. Therefore the slip velocity at the wall is obtained by equating the exerted tangential force on the wall and the particle shear stress close to the wall. The granular temperature at the wall is determined by equating the wall granular temperature flux to the summation of the inelastic dissipation of energy and the generation of granular energy resulting from slip at the wall. No material is permitted to pass through the wall boundaries.

Figure 3.4 No slip wall boundary condition
3.4 Initial Conditions

Initial conditions typically are not of interest because solutions are dependent on boundary conditions; however, initial conditions must be specified as realistic values to promote convergence. The two initial conditions that must be specified in the bed region and the freeboard are the gas and solids velocities, and the volume fractions of each phase. The bed is modeled as a homogeneous mixture with uniform bulk density and void fraction. The initial gas velocity specified throughout the bed \( U_{g,0} \) is solved by balancing the volumetric flow rate entering the reactor, \( Q = AU_g \), and the volumetric flow rate through the bed that has both granular material and gas. Equating both flow rates:

\[
AU_g = A_g U_{g,0} \tag{61}
\]

where \( A \) is the cross sectional area of the reactor, \( U_g \) is the inlet superficial gas velocity, and \( A_g \) is the cross sectional area occupied by gas in the bed. The gas volume fraction in the bed mixture can be defined as the ratio of the volume occupied by the gas, \( V_g \), over the total bed volume, \( V_T \):

\[
\varepsilon_g = \frac{V_g}{V_T} = \frac{A_g h_{bed}}{Ah_{bed}} = \frac{A_g}{A} \tag{62}
\]

Combining equation (61) and equation (62) and solving for \( U_{g,0} \):

\[
U_{g,0} = \frac{U_g}{\varepsilon_g} \tag{63}
\]

The initial gas velocity in the bed is specified using equation (63).

The freeboard is initially modeled with a void fraction of unity, meaning the freeboard is only occupied by the gas phase. The initial gas velocity in the freeboard is equal to the inlet gas velocity, \( U_g \). The boundary conditions and initial conditions used to model a fluidized bed are shown in Figure 3.5.
Figure 3.5 Fluidized bed reactor modeling (a) boundary conditions and (b) initial conditions.
Chapter 4 Two-Stage Reactor

In this chapter, a two-stage reactor is modeled to determine the fluidizing characteristics of a binary mixture. Two-stage reactors differ from single-stage reactors because they do not maintain a constant diameter, but instead increase in diameter over an expansion region. Two-stage geometries will be discussed more thoroughly, later in this chapter. A grid resolution study is performed to ensure the MFIX simulations are relatively grid insensitive. Motivation and details of the reactor geometry and binary mixture are presented next. Experimental pressure drop data is initially compared to MFIX simulations for a single-stage geometry to validate the MFIX model. The two-stage reactor is then modeled and validated using experimental data. The two-stage reactor operation is studied using MFIX for varied inlet gas velocities. The key consideration in the operation of the two-stage geometry is segregation of the binary mixture. It should be noted that the experimental reactor is made of stainless steel, therefore Kaolin instead of sand is used as the inert material.

4.1 Grid Resolution Study

A simple single-stage geometry is used for the grid validation study. The geometry is a cylindrical domain with a 7.62 cm diameter and 25.4 cm height above the distributor plate. A grid resolution study is performed for a single-component system of Kaolin using the simple reactor geometry and particle properties shown in Figure 4.1. Kaolin is an inert granular material similar to sand, but is less abrasive on the reactor walls. The domain is discretized using a coarse mesh (15×50), medium mesh (30×100), and fine mesh (60×200) using square cells with side lengths of 0.508 cm, 0.254 cm, and 0.127 cm, respectively. The number of cells, cell size, computational time (CPU), number of time steps, average time step, and computational
time required per time step for each cell are presented in Table 4.1. The results presented for the three meshes are time averaged from 5 s to 40 s at intervals of 0.01 s with 3,500 time realizations.

![Figure 4.1 Schematic of grid resolution geometry](image)

Table 4.1 Grid resolution and central processing unit information

<table>
<thead>
<tr>
<th>Mesh</th>
<th>15×50</th>
<th>30×100</th>
<th>60×200</th>
</tr>
</thead>
<tbody>
<tr>
<td># Cells</td>
<td>750</td>
<td>3000</td>
<td>12000</td>
</tr>
<tr>
<td>Cell Size (cm × cm)</td>
<td>0.508 × 0.508</td>
<td>0.254 × 0.254</td>
<td>0.127 × 0.127</td>
</tr>
<tr>
<td>CPU (s)</td>
<td>1.981</td>
<td>26,803</td>
<td>360,886</td>
</tr>
<tr>
<td># Time-Steps</td>
<td>16,196</td>
<td>42,790</td>
<td>145,980</td>
</tr>
<tr>
<td>Average Δt (s)</td>
<td>0.0024</td>
<td>0.00093</td>
<td>0.00027</td>
</tr>
<tr>
<td>µs/Time-Step/Cell</td>
<td>163</td>
<td>209</td>
<td>206</td>
</tr>
</tbody>
</table>

\( m = 365 \text{ g} \)
\( D = 348 \text{ µm} \)
\( \rho = 2.0 \text{ (g/cm}^3\text{)} \)
\( \varepsilon_g = 0.38 (-) \)

\( m = 365 \text{ g} \)
\( D = 348 \text{ µm} \)
\( \rho = 2.0 \text{ (g/cm}^3\text{)} \)
\( \varepsilon_g = 0.38 (-) \)

\( U_g = 9.0 \text{ cm/s} \)
Void fraction profiles at vertical heights of 2 cm and 4 cm are compared in Figure 4.2. The void fraction is representative of the volume fraction occupied by the gas phase. When void fraction values are small, a high percentage of the volume is occupied by Kaolin, and when void fraction values are large, a high percentage of the volume is occupied by gas. Examination of the profiles in Figure 4.2a at a height of 2 cm show a general agreement between all three meshes that the void fraction is fairly homogeneous. Examination of the profiles in Figure 4.2b at a height of 4 cm shows small variations between the medium and fine meshes, while the coarse mesh differs greatly. At a height of 4 cm, the fine and medium meshes show an increased amount of Kaolin near the walls with an adjacent region containing an increased amount of gas approximately, 1 cm inside the walls. However the coarse mesh does not capture these wall effects and shows a more homogeneous distribution of gas and Kaolin.

![Graph](image)

Figure 4.2 Void fraction versus horizontal location comparing three meshes coarse, medium and fine at vertical heights of (a) 2 cm and (b) 4 cm.
Spatially averaging the void fraction at each vertical location in the domain and plotting them versus the reactor height, $Z$, for the three meshes is shown in Figure 4.3a. When the void fraction equals unity the volume is completely occupied by gas. These profiles allow the bed expansion height and average solids volume distribution to be determined. Upon examining the profiles in Figure 4.3a, there is no noticeable difference between the fine and medium meshes, while the coarse mesh differs greatly where the bed begins to expand between 5 cm - 7 cm. The fine and medium meshes predict a bed expansion height of 6.5 cm, which is confirmed by viewing the void fraction contours for the medium mesh shown in Figure 4.3b, while the coarse mesh predicts a lower bed expansion height closer to 6 cm.

Vertical gas velocity profiles at vertical heights of 2 cm and 4 cm are also compared in Figure 4.4. At the lower height of 2 cm all the meshes show a more homogeneous vertical gas velocity as shown in Figure 4.4a. Examination of the profiles in Figure 4.4b shows small variations between the medium and fine meshes at a height of 4 cm, while the coarse mesh differs greatly.

![Figure 4.3](image-url)  
(a) Time and horizontally averaged void fraction versus vertical height for three meshes coarse, medium and fine. (b) Time averaged void fraction contour plot for medium mesh.
Richardson’s extrapolation of the void fraction and vertical gas velocity produces average relative errors within ±1% for the medium mesh. The medium mesh is also less computationally expensive as shown in Table 4.1. Therefore, the medium mesh will be used for a majority of the following cases, and when the smaller two-stage reactor geometry is modeled the fine mesh will be used. MFIX is used to study the hydrodynamics and segregation in a non-reactive two-stage geometry. The goal is to determine the amount of each material and gas velocity to produce segregation to help the experimentalists achieve proper conditions. To validate the MFIX parameters, a simple single-stage geometry is modeled and compared to experimental pressure drop data (Section 4.2) and then a parametric study is performed for the two-stage reactor (Section 4.3).
4.2 Initial Validation of MFIX Model

The initial model used to validate MFIX is a single-stage geometry shown in Figure 4.1. The geometry and particle properties, initial conditions and all pressure data were measured by Dr. F. Agblevor’s research team in the Department of Biological Systems Engineering at Virginia Tech. Three cases are validated using the single-stage reactor model and the case properties are listed in Table 4.2. Case 1 is a simple single-component system used to validate the Kaolin particle properties, while case 2 and case 3 are more complicated binary mixtures. Case 2 and case 3 differ in the amount of FCC present in the binary mixture.

MFIX was used to model case 1 using the properties and conditions shown in Table 4.2. The MFIX predictions for pressure drop versus inlet gas velocity are compared to the experimental data in Figure 4.5. As discussed in Section 2.1, the bed pressure drop increases linearly with inlet gas velocity until fluidization at $U_{mf} = 7$ cm/s. Figure 4.5 shows very good agreement between the MFIX simulations and the experimental data.

For the binary system of case 2, the MFIX predictions for pressure drop compare well to the experimental data shown in Figure 4.6a, accurately predicting minimum fluidization velocity $U_{mf} = 6.4$ cm/s. Likewise, predictions of the binary system of case 3 (Figure 4.6b) that contains more FCC show excellent agreement between the simulations and experiments, where $U_{mf} = 6.4$ cm/s.

<table>
<thead>
<tr>
<th>Case</th>
<th>Kaolin Mass (g)</th>
<th>FCC Mass (g)</th>
<th>Kaolin Characteristic Diameter (µm)</th>
<th>FCC Characteristic Diameter (µm)</th>
<th>Kaolin Density (g/cm³)</th>
<th>FCC Density (g/cm³)</th>
<th>Mixture ε_{mf,g} (-)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>365</td>
<td>-</td>
<td>348</td>
<td>-</td>
<td>2.0</td>
<td>-</td>
<td>0.38</td>
</tr>
<tr>
<td>2</td>
<td>354</td>
<td>306</td>
<td>348</td>
<td>58</td>
<td>2.0</td>
<td>2.0</td>
<td>0.36</td>
</tr>
<tr>
<td>3</td>
<td>354</td>
<td>218</td>
<td>348</td>
<td>58</td>
<td>2.0</td>
<td>2.0</td>
<td>0.36</td>
</tr>
</tbody>
</table>
The three cases presented here validate that the particle properties and MFIIX models are correct for a binary mixture of Kaolin and FCC. The more complicated two-stage reactor geometry can now be modeled using MFIIX.

Figure 4.5 Case 1, single-component system composed of 365 g Kaolin comparing pressure drop from experiments and MFIIX simulations.

Figure 4.6 Binary system comparing pressure drop from experiments and MFIIX simulations for (a) Case 2, 354 g Kaolin and 306 g FCC and (b) Case 3, 354 g Kaolin and 218 g FCC
4.3 Two-Stage Reactor

Pyrolysis in fluidized beds requires high heat transfer rates to volatilize solid fuels such as biomass. Inert bed materials, e.g., sand or Kaolin, are typically used to provide the necessary heat transfer. In order to produce a higher quality bio-oil, it is desirable to use fluid catalytic cracking (FCC) materials to control the chemical reactions. It is therefore important to incorporate both inert bed materials and FCC materials in the pyrolysis process. To incorporate these two materials in a single reactor, the inert bed material and FCC must be maintained in separate regions of the reactor. One method to maintain separate material regions is to design the reactor to produce segregation between the inert material and the FCC. Two-stage reactors, like single-stage reactors, are typically cylindrical. However the two-stage reactor has two distinct reactor diameters, as shown in Figure 4.7 for the reactor design by Dr. F. Agblevor. In most cases, the two stages are connected with an expansion region. The design of the two-stage reactor aims to increase segregation between the inert material and the FCC by expanding the reactor diameter in order to reduce the vertical gas velocity. The smaller diameter of the lower region should fluidize both the inert material and FCC, while the larger diameter of the upper region should only fluidize the FCC. Therefore, the upper stage of the reactor would only contain FCC while the lower stage would predominantly contain the inert material.
The first issue in the operation of a two stage reactor is determining appropriate amounts of bed material. In order to limit the expansion of the inert bed material (Kaolin) to only fluidize in the lower stage of the reactor, it is necessary to run several preliminary simulations with Kaolin only, as summarized in Table 4.3. Using 25 g of Kaolin, the initial bed height was 6.0 cm and after the fluidization the bed expanded to an average height of 11.1 cm, which was within the first stage region. For 36 g of Kaolin, the initial bed height was 8.0 cm and after fluidization the bed expanded to an average height of 11.9 cm. The bed expansion was too close to the second stage region; therefore, the mass of Kaolin for the remainder of the simulations will be fixed at 25 g.

Table 4.3. Determination of appropriate Kaolin mass.

<table>
<thead>
<tr>
<th>Kaolin mass (g)</th>
<th>Inlet velocity (cm/s)</th>
<th>Initial bed height (cm)</th>
<th>Expansion bed height (cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>34.32</td>
<td>6.0</td>
<td>11.11</td>
</tr>
<tr>
<td>36</td>
<td>34.32</td>
<td>8.0</td>
<td>11.89</td>
</tr>
</tbody>
</table>
The particle properties used for the remainder of the simulations are shown in Table 4.4. The properties of Kaolin and FCC differ advantageously for the promotion of bed segregation. Kaolin has a larger diameter and higher density than the FCC, which should promote desirable size and density segregation of the Kaolin to the first stage (lower) region. The propensity for segregation can also be appreciated by examining the predicted individual minimum fluidization velocities \( U_{mf} \) of each material, where FCC fluidizes more readily at a lower velocity (see Table 4.4). MFIX simulations were used to predict the pressure drop curve for the Kaolin-FCC mixture over a range of inlet velocities. The minimum fluidization velocity for the binary mixture is approximately \( U_{mf} = 9.3 \) cm/s.

To determine the inlet gas velocity that produces the maximum bed segregation, four simulations were performed at varied inlet gas velocities. All inlet velocities were based on the minimum fluidization of the mixture. A minimum fluidization void fraction of 0.69 was used for each case, where the inlet velocities correspond to \( 1.3U_{mf} \), \( 2.4U_{mf} \), \( 3.6U_{mf} \), and \( 4.8U_{mf} \). Figure 4.8a shows the expansion of the bed by analyzing void fraction versus height in the reactor. As the inlet velocity increases, more gas is present in the lower portion of the reactor, i.e., below 10 cm, and varies from \( \varepsilon_g = 0.78 \) at \( 1.3U_{mf} \) to \( \varepsilon_g = 0.88 \) at \( 4.8U_{mf} \). The nonuniform void fraction is indicative of a more turbulent-like fluidized bed as shown by Xie et al. [49]. Another feature is the drop in void fraction at a height of 10 cm at the point where the reactor expands, shown in Figure 4.8b. As the reactor diameter expands, the gas velocity begins to decrease resulting in lower particle drag forces and less bed expansion. Therefore, the void fraction in the expansion region is the lowest as compared to the amount of gas present in the first and second stages.
Table 4.4. Particle properties for binary mixture.

<table>
<thead>
<tr>
<th>Particle</th>
<th>Mass (g)</th>
<th>Diameter (µm)</th>
<th>Density (g/cm³)</th>
<th>Bulk Density (g/cm³)</th>
<th>U_{mf} (cm/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Kaolin</td>
<td>25</td>
<td>99.2</td>
<td>2.9</td>
<td>0.24</td>
<td>11.24</td>
</tr>
<tr>
<td>FCC</td>
<td>50</td>
<td>58.5</td>
<td>2.2</td>
<td>0.49</td>
<td>2.96</td>
</tr>
</tbody>
</table>

Figure 4.8  (a) Void fraction versus vertical height for various inlet velocities (as a function of \( U_{mf} \)). (b) Reactor geometry.

Void fraction alone does not demonstrate that the bed has segregated, but can suggest segregation. To be sure that the two bed materials are segregating, it is necessary to examine individual particle volume fractions, as demonstrated by the contour of void fraction, volume fraction of Kaolin and volume fraction of FCC, shown in Figure 4.9. Two inlet gas velocities of 1.3\( U_{mf} \) (Figure 4.9a-c) and 3.6\( U_{mf} \) (Figure 4.9d-f) are compared and analyzed for the presence of desirable segregation. It is apparent by comparing (a) and (d) that the gas phase becomes more dominant in the lower stage of the reactor at the higher inlet gas velocity. For both inlet gas velocities, the majority of the granular material is displaced to the sides of the sloping walls of
the expansion region, represented as the light green regions in (a) and (d). For an inlet gas velocity of $1.3U_{mf}$, Kaolin is present in the lower stage of the reactor and also along the lower portion of the expansion side walls, light blue, shown in (b) while FCC predominantly resides along the upper portion of the sloping expansion walls, orange and yellow, shown in (c).

An inlet gas velocity of $1.3U_{mf}$ suggests that it will promote a reasonably sized, highly fluidized preheat zone in the lower stage of the reactor, while also providing a slower velocity region to allow long contact time between the gases and FCC in the upper stage of the reactor. At higher inlet gas velocities, such as $3.6U_{mf}$, the presence of segregation along the expansion side walls decreases (see Figure 4.9 (e) and (f)), while the lower stage preheat region is greatly reduced due to elutriation of Kaolin and FCC.

It can be concluded that operation of a two-stage reactor is highly dependent upon the inlet gas velocity. For this particular geometry and binary mixture, operation is optimized at an inlet gas velocity of $1.3U_{mf}$. However each reactor geometry and binary mixture will require different operation conditions to promote segregation. The work presented here was a preliminary step in helping the experimental team to determine the operating conditions for their reactor. However, other questions were raised; specifically, is it possible to predict fluidization characteristics analytically, without a full CFD analysis? The next chapter shows how a new model was developed to enhance the understanding of fluidization of any mixture. Chapter 6 will then revisit the work described in chapter 4.
Figure 4.9 Time averaged contours of volume fractions for inlet gas velocity of $1.3U_{mf}$ (a) gas, (b) Kaolin, and (c) FCC. Inlet gas velocity of $3.6U_{mf}$ (d) gas, (e) Kaolin, and (f) FCC.
5.1 MASS Method Theory

The motivation for the new method is based on previously published experimental studies by Formisani et al. [1, 2] that identified unique fluidization characteristics of fluidizing beds. The granular material consisted of glass beads, which formed a multi-component system of beads of varying diameters. Measurements of pressure across the bed with increasing gas velocity were recorded to produce the pressure drop curves and to determine $U_{mf}$. Formisani et al. [1, 2] also calculated the minimum fluidization velocity for the multi-component bed using mass-weighted mixture properties and single-component correlations. Their calculations under-predicted the experimentally determined minimum fluidization velocities. However, it was noted that the initial slope of the pressure drop curve could be predicted from the slope of a line intersecting the origin and the point corresponding to the calculated minimum fluidization velocity and total pressure drop ($U_{mf,M}, \Delta P_T$). These experimental observations are the basis of the new method, which will be referred to as the Mass Accounting in the Stationary System (MASS) method for the remainder of this work.

Formisani et al.’s studies [1, 2] support the theory that the slope of pressure drop versus inlet gas velocity is equal to the difference between the total pressure drop, $\Delta P_T$, and the current pressure drop, $\Delta P$, divided by the difference between the predicted mixture minimum fluidization velocity, $U_{mf,M}$, and the current inlet velocity, $U$. A way to express the slope mathematically is:

$$\frac{\partial \Delta P}{\partial U} = \frac{\Delta P_T - \Delta P}{U_{mf,M} - U} \quad (64)$$
where the total pressure drop is calculated using equation (2) and \( U_{mf,M} \) can be calculated using equation (7) with the definitions of mixture density and diameter using Method 2 found in Table 2.3:

\[
\rho_M = \left[ \sum_{i=1}^{n} \left( \frac{X_i}{\rho_i} \right) \right]^{-1}
\]

(65)

\[
D_M = \left[ \rho_M \sum_{i=1}^{n} \left( X_i / (\rho_i D_i \varphi_i) \right) \right]^{-1}
\]

(66)

for a system of \( n \) components.

The total mass of a multi-component system does not change, however the amount of mass that fluidizes does change depending on the inlet gas velocity. Thus, the mass that remains stationary should be used to determine the mass fraction of a mixture component property, and can be expressed by the novel definition of mass fraction for a fluidizing system as:

\[
X_i = \frac{m_i - \frac{A\Delta P_i}{g}}{m - \frac{A\Delta P}{g}}
\]

(67)

where \( \Delta P_i \) is the component contribution to the current pressure drop, \( \Delta P \). As inlet gas velocity increases, particles in the system corresponding to different components begin to fluidize depending on the particle density and diameter. equation (67) accounts for the mass that has fluidized \( (A\Delta P_i/g) \) by subtracting this mass from the initial mass, \( m_i \), present in the stationary bed for each component. Therefore, the mass fraction of the stationary bed changes as a function of inlet gas velocity.

The final part of the analysis is to determine what portion of the pressure drop, \( \Delta P \), is due to each component, \( \Delta P_i \). For multi-component systems, the solids density in equation (5) can be
replaced with the mixture density, whereby, solving Equation (66) for $\rho_M$ and substituting into equation (5) yields:

$$\Delta P_T = \varepsilon_r \rho_M g h_0 = \frac{\varepsilon_r g h_0}{D_M \sum_{i=1}^{n} \left( X_i \left( \frac{\rho_i D_i \psi_i}{\rho_M} \right) \right)}$$  \hspace{1cm} (68)

Upon rearranging equation (68):

$$1 = \sum_{i=1}^{n} \left( \frac{D_M}{D_i \psi_i} \right) \left( \frac{\rho_M}{\rho_i} \right) X_i$$  \hspace{1cm} (69)

which can be interpreted as the summation of the ratios of the component contribution to the pressure drop over the total pressure drop:

$$1 = \sum_{i=1}^{n} \frac{\Delta P_i}{\Delta P_T}$$  \hspace{1cm} (70)

Assuming that the properties of the bed are represented by the unfluidized components, and equating equation (69) and (70):

$$\frac{\Delta P_i}{\Delta P_T} = \left( \frac{D_M}{D_i \psi_i} \right) \left( \frac{\rho_M}{\rho_i} \right) X_i$$  \hspace{1cm} (71)

The relationship in equation (64) can now be used with single-component correlations for $U_{mf}$ to determine the behavior of any multi-component system. With a complete set of equations, the pressure drop can be calculated as a function of inlet gas velocity and particle properties using the novel approach. By considering how much mass is fluidized at a particular inlet gas velocity, the equations must now be discretized with respect to the inlet gas velocity to incorporate mixture property changes.

Equation (64) is discretized using a first-order Taylor series expansion to represent the slope of pressure drop with respect to inlet gas velocity:
\[
\frac{\partial \Delta P_i^k}{\partial U} = \frac{\Delta P_i^{k+1} - \Delta P_i^k}{U_i^{k+1} - U_i^k}
\] (72)

where the superscript \( k \) is the discretization index corresponding to the inlet gas velocity \( U \).

Figure 5.1 represents how different components in a system fluidize until the entire system fluidizes with a total pressure drop \( \Delta P_T \). Substituting Equation (72) into Equation (64) and solving for the unknown pressure, \( \Delta P^{k+1} \):

\[
\Delta P^{k+1} = \Delta P^k + \left( \frac{\Delta P_T - \Delta P^k}{U_{mf,M}^k - U_i^k} \right) \left( U_i^{k+1} - U_i^k \right)
\] (73)

Equation (73) represents the prediction of the next pressure drop value based on the current pressure drop, \( \Delta P^k \), the step size for inlet gas velocity \( (U_i^{k+1} - U_i^k) \) and the current mixture minimum fluidization velocity, \( U_{mf,M}^k \).

![Figure 5.1 Pressure drop versus inlet gas velocity showing discretization scheme for the mixture and components.](image)

At each new inlet gas velocity, \( k+1 \), it is necessary to calculate each component pressure drop as shown in Figure 5.1. To determine the component pressure drop, Equation (71) is discretized:
\[ \Delta P_i^{k+1} = \Delta P_i^k + X_i^k(\Delta P^{k+1} - \Delta P^k) \left( \frac{D_M^k}{D_i \psi_i} \left( \frac{\rho_M^k}{\rho_i} \right) \right) \]  

(74)

Each component pressure drop can be used to calculate \( X_i \) by discretizing equation (67):

\[ X_i^{k+1} = \frac{m_i - A\Delta P_i^{k+1}}{g} \frac{A\Delta P_i^{k+1}}{g} \]  

(75)

The component mass fractions can then be used to solve for the mixture properties using the discretized forms of equations (65) and (66).

\[ \rho_M^{k+1} = \left[ \sum_{i=1}^{n} \left( \frac{X_i^{k+1}}{\rho_i} \right) \right]^{-1} \]  

(76)

\[ D_M^{k+1} = \left[ \rho_M^{k+1} \sum_{i=1}^{n} \left( \frac{X_i^{k+1}}{\rho_i D_i \psi_i} \right) \right]^{-1} \]  

(77)

and equations (76) and (77) are then used to solve for the mixture minimum fluidization velocity by discretizing Equation (7):

\[ U_{mf,M}^{k+1} = \frac{(D_M^{k+1})^2(\rho_M^{k+1} - \rho_g)g}{150 \mu_g} \frac{e_{mf,g}^3}{(1 - e_{mf,g})} \]  

Re_{mf} < 20

(78)

Using the initial condition that the pressure drop is zero at zero velocity, it is possible to iterate equations (74) through (78) to solve for the pressure drop versus inlet gas velocity.

5.2 Results and Discussion

The MASS method will be validated with experimental data published in the literature as well as computational fluid dynamics (CFD) simulations performed using MFIX. The authors have extensively used MFIX and further details are discussed in their previous work [10, 48,49]. A total of 9 cases will be presented and a summary of the properties are listed in Table 5.1.
Table 5.1 Properties of each case (mass, diameter, density, void fraction and reactor cross-sectional area).

<table>
<thead>
<tr>
<th>Case</th>
<th>$m_1$ (g)</th>
<th>$m_2$ (g)</th>
<th>$m_3$ (g)</th>
<th>$\psi D_1$ (µm)</th>
<th>$\psi D_2$ (µm)</th>
<th>$\psi D_3$ (µm)</th>
<th>$\rho_1$ (g/cm$^3$)</th>
<th>$\rho_2$ (g/cm$^3$)</th>
<th>$\rho_3$ (g/cm$^3$)</th>
<th>$\varepsilon_{g,mf}$</th>
<th>$A_c$ (cm$^2$)</th>
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</thead>
<tbody>
<tr>
<td>1</td>
<td>1180</td>
<td>-</td>
<td>-</td>
<td>495</td>
<td>-</td>
<td>2.6</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.373</td>
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</tr>
<tr>
<td>2</td>
<td>488</td>
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<td>-</td>
<td>499</td>
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<td>2.53</td>
<td>-</td>
<td>-</td>
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<tr>
<td>3</td>
<td>458</td>
<td>1458</td>
<td>-</td>
<td>499</td>
<td>271</td>
<td>2.53</td>
<td>2.53</td>
<td>-</td>
<td>-</td>
<td>0.382</td>
<td>80.12</td>
</tr>
<tr>
<td>4</td>
<td>437</td>
<td>437</td>
<td>375</td>
<td>517</td>
<td>392</td>
<td>322</td>
<td>2.71</td>
<td>2.71</td>
<td>2.71</td>
<td>0.418</td>
<td>64.0</td>
</tr>
<tr>
<td>5</td>
<td>491</td>
<td>491</td>
<td>246</td>
<td>517</td>
<td>392</td>
<td>322</td>
<td>2.71</td>
<td>2.71</td>
<td>2.71</td>
<td>0.423</td>
<td>64.0</td>
</tr>
<tr>
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<td>539</td>
<td>539</td>
<td>120</td>
<td>517</td>
<td>392</td>
<td>322</td>
<td>2.71</td>
<td>2.71</td>
<td>2.71</td>
<td>0.434</td>
<td>64.0</td>
</tr>
<tr>
<td>7</td>
<td>300</td>
<td>100</td>
<td>50</td>
<td>200</td>
<td>400</td>
<td>600</td>
<td>2.0</td>
<td>2.0</td>
<td>2.0</td>
<td>0.3</td>
<td>45.6</td>
</tr>
<tr>
<td>8</td>
<td>300</td>
<td>100</td>
<td>50</td>
<td>400</td>
<td>400</td>
<td>400</td>
<td>4.0</td>
<td>2.0</td>
<td>0.5</td>
<td>0.3</td>
<td>45.6</td>
</tr>
<tr>
<td>9</td>
<td>50</td>
<td>100</td>
<td>300</td>
<td>600</td>
<td>400</td>
<td>200</td>
<td>0.5</td>
<td>2.0</td>
<td>4.0</td>
<td>0.3</td>
<td>45.6</td>
</tr>
</tbody>
</table>

The first six cases will compare the MASS method with both experimental results and MFIx, while the last three cases will compare the MASS method only with MFIx.

The first case (1) considers a fluidized bed of glass beads modeled as a single-component system and the experimental data is from the work of Franka et al. [3]. The initial fluidization void fraction, $\varepsilon_{mf,g}$, was determined from the experimental data for the material at rest in the reactor. Figure 5.2 presents the change in pressure as the inlet gas velocity increases, comparing the experiments with MFIx and the MASS method. The MASS method predicts a linearly increasing pressure drop and a minimum fluidization velocity that compares well with both the experimental data and MFIx simulations. The horizontal dotted line in Figure 5.2 is the pressure drop calculated using equation (2) and assumes the entire bed is fluidized, which is identical to the MASS method and simulations.
Cases 2 and 3 represent a special case of a multi-component system that can be described by two components called a binary mixture. The difference between these two cases is that a larger diameter particle is used to model the second component in case 3. The experimental data are from the work of Formisani et al. [2] for a glass bead bed composed of two characteristic particle diameters. The void fraction $\varepsilon_{mf,g}$ was experimentally measured for a stationary bed using two methods. The first method measured the stationary bed void fraction after the bed was carefully mixed and poured into the reactor. The second method measured the stationary bed void fraction after the bed was fluidized and then rapidly defluidized. Each experimental method produced different values for the minimum fluidization void fraction. As shown in Figure 5.3, the MASS method accurately predicts $U_{mf}$ and pressure drop measured in the experiments and predicted using MFIX when $\varepsilon_{mf,g}$ corresponds to the experimental value obtained by carefully pouring the mixture into the reactor.
Figure 5.3 Binary mixture pressure drop versus inlet gas velocity comparing experiments, MFIX and MASS method for glass beads with (a) case 2 composed of 499 µm and 172 µm diameter particles and (b) case 3 composed of 499 µm and 271 µm diameter particles [2].

Cases 4, 5 and 6 represent ternary mixtures that are modeled with three characteristic-components whereby each case differs in the initial mass fractions of each component. The experimental data for these cases come from the work of Jena et al. [4] for a bed consisting of dolomite of various diameters. Jena et al. reported void fraction at fluidization and calculated sphericity of the dolomite particles using a correlation developed by Narsimhan et al. [50]. The MASS method compares very well with the experimental data and MFIX simulations shown in Figure 5.4, and demonstrates the ability of the MASS method to capture the fluidization physics of the multi-component systems.
Cases 7-9 represent arbitrary multi-component systems and are intended to demonstrate the ability of the MASS method to predict more complex systems. Each case is represented as a three-component system and each system has the same total bed mass of 450 g and initial solids packing of 0.7 (i.e., $\varepsilon_{mf,g} = 0.3$), which assumes a well-packed bed. Case 7 models a system of particles of the same density but each component has a unique diameter to represent three...
particle size distributions of different fractions. Case 8 models a system where the particle diameters are the same but each component represents a unique density. The last case (9) is a completely nonhomogenous system relative to particle density, size and mass. Cases 7-9 are compared to the computational results predicted by MFI in Figure 5.5(a-c), where overall, there is excellent agreement between the MASS method and the simulations.

![Figure 5.5](image)

Figure 5.5 Ternary mixture pressure drop versus inlet gas velocity comparing experiments, MFI and MASS method for (a) cases 7, (b) case 8, and (c) case 9.
As discussed previously, the minimum fluidization velocity is determined by noting when the pressure drop through the bed no longer increases with increasing gas velocity. The value of $U_{mf}$ can be determined through a visual inspection of the pressure drop curve. As suggested by Geldart [12], a straight line can be used to capture the initial slope of the pressure drop and a horizontal line can be used to capture the average pressure drop after fluidization. The intersection of the two lines identifies the minimum fluidization velocity. However, as can be seen in Figure 5.3-Figure 5.5, the pressure drop may asymptotically change near the point of fluidization until the flow is fully fluidized, and so care must be taken to determine the approximate lines that represent a majority of the data. The $U_{mf}$ values reported in the literature, whether from experiments or CFD, may include some error from either the estimation of $U_{mf}$ or the techniques (experimental or numerical error) used to obtain pressure drop.

The MASS method can also be used to determine the minimum fluidization velocity based on the pressure drop trends. Referring to Figure 5.3 and Figure 5.4, the pressure drop appears to be relatively constant above the minimum fluidization velocity, consistent with the experiments. However, not readily visible is a slight (asymptotic) increase in pressure drop until 100% of the mass is fluidized. In reality, no experiment is perfect and therefore 100% of the mass in the bed will never fluidize due to distributor plate configuration or electric static build-up along the reactor walls or even the material used [51, 52]. Therefore, the MASS method can predict $U_{mf}$ after a criterion is established for the percent of mass that typically fluidizes, which is equal to a percentage of the total pressure drop. Table 5.2 presents $U_{mf}$ for the MASS method by consider 97, 98, 99 and 100% of the total pressure drop, and is compared with the experiments (cases 1-6)
and MFIX predictions (cases 1-9). Assuming that 98% of the bed is fluidized, the predicted $U_{mf}$ from the MASS method provides very good results with an average relative error of ±4%.

Table 5.2 Minimum fluidization velocities at various percents of total pressure drop for the MASS method to compare to experimental and MFIX results.

<table>
<thead>
<tr>
<th>Case</th>
<th>$U_{mf,97%}$ (cm/s)</th>
<th>$U_{mf,98%}$ (cm/s)</th>
<th>$U_{mf,99%}$ (cm/s)</th>
<th>$U_{mf,100%}$ (cm/s)</th>
<th>MFIX $U_{mf,M}$ (cm/s)</th>
<th>Experiment $U_{mf,M}$ (cm/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>18.6</td>
<td>18.8</td>
<td>19.0</td>
<td>19.2</td>
<td>18.0</td>
<td>19.9</td>
</tr>
<tr>
<td>2</td>
<td>9.9</td>
<td>11.6</td>
<td>13.9</td>
<td>17.0</td>
<td>12.0</td>
<td>11.0</td>
</tr>
<tr>
<td>3</td>
<td>11.0</td>
<td>12.0</td>
<td>13.6</td>
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<td>12.0</td>
<td>12.0</td>
</tr>
<tr>
<td>4</td>
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<td>24.0</td>
<td>25.3</td>
<td>32.9</td>
<td>25.0</td>
<td>22.6</td>
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<td>25.4</td>
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<td>26.0</td>
<td>25.6</td>
</tr>
<tr>
<td>6</td>
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<td>30.0</td>
<td>31.2</td>
<td>37.9</td>
<td>26.0</td>
<td>28.7</td>
</tr>
<tr>
<td>7</td>
<td>4.2</td>
<td>4.8</td>
<td>5.8</td>
<td>10.1</td>
<td>6.0</td>
<td>-</td>
</tr>
<tr>
<td>8</td>
<td>8.3</td>
<td>8.5</td>
<td>8.7</td>
<td>9.0</td>
<td>9.0</td>
<td>-</td>
</tr>
<tr>
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<td>2.8</td>
<td>2.8</td>
<td>2.8</td>
<td>2.8</td>
<td>2.8</td>
<td>-</td>
</tr>
</tbody>
</table>

It should be noted that comparing MFIX to the experiments also is within ±7%. For the remaining discussion and presentation of results, the $U_{mf}$ predicted by the MASS method will be based on calculations when the pressure drop is 98% of the total pressure drop.

As discussed, the published literature has numerous studies that report correlations for minimum fluidization velocity but it is not clear if they can be used to predict $U_{mf}$ when a bed medium is heterogeneous. Thus, mixture properties are used with these correlations in an effort to better predict the fluidization characteristics. Section 2.2 and 2.3 summarize many of these relationships, which are shown in Table 2.1 - Table 2.3. It is therefore worthwhile to test how well these correlations perform for multi-component systems and compare with the experiments, MFIX and the MASS method. The cases selected include representing the bed as: a single material (case 1), a binary mixture (case 3) and a ternary mixture (case 4). Table 5.3 summarizes the values of $U_{mf}$ for many of the correlations listed in the previous tables. To complement the data in Table 5.3, Figure 5.6 presents the three cases comparing the experimentally measured
minimum fluidization velocity $U_{mf,exp}$ with the correlation predictions, MFIX and the MASS method for $U_{mf,predict}$. The solid line represents perfect agreement between the experiments and predictions, the dashed line (−−−) identifies values within ±10% relative error and the dashed-dotted line (−⋯−) identifies values within ±15% relative error. Table 5.3 shows all correlations that are within ±15% error with an italicized number.

Table 5.3 Predicted $U_{mf,predict}$ (cm/s) for cases 1, 3 and 4. Italicized numbers are ±15% relative error.

<table>
<thead>
<tr>
<th>Method</th>
<th>Case 1</th>
<th>Case 3</th>
<th>Case 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Experiment $U_{mf,exp}$ (cm/s)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MFIX simulations</td>
<td>18.0</td>
<td>12.0</td>
<td>25.0</td>
</tr>
<tr>
<td>MASS method</td>
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<td>12.0</td>
<td>24.0</td>
</tr>
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<td>7.7</td>
<td>19.7</td>
</tr>
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<td>Investigators listed in Table 1</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>Babu, Shah &amp; Talwalkar [19]</td>
<td>36.2</td>
<td>15.5</td>
<td>26.6</td>
</tr>
<tr>
<td>Bourgeois &amp; Grenier [20]</td>
<td>22.7</td>
<td>9.2</td>
<td>16.3</td>
</tr>
<tr>
<td>Chitester [21]</td>
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<td>10.6</td>
<td>18.7</td>
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<td>Grace [22]</td>
<td>22.9</td>
<td>9.3</td>
<td>16.4</td>
</tr>
<tr>
<td>Richardson &amp; St. Jeromino [23]</td>
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<td>8.8</td>
<td>15.5</td>
</tr>
<tr>
<td>Saxena &amp; Vogel [24]</td>
<td>32.4</td>
<td>13.7</td>
<td>23.6</td>
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<td>Thonglimp [25]</td>
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<td>8.4</td>
<td>14.9</td>
</tr>
<tr>
<td>Wen &amp; Yu [18]</td>
<td>19.2</td>
<td>7.6</td>
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<td>Zhiping [26]</td>
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<td>17.1</td>
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<td>7.4</td>
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<td>10.0</td>
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<td>9.1</td>
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<td>Pillai &amp; Raja Rao [37]</td>
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<td>8.9</td>
<td>16.5</td>
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<td>Riba, Routie &amp; Couderc [38]</td>
<td>30.3</td>
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Figure 5.6 Predicted $U_{mf,\text{predict}}$ versus experimental $U_{mf,\text{expt}}$ for cases 1, 3 and 4 for (a) all data, (b) case 3, and (c) cases 1 and 4. Dashed lines (– – –) ±10% and (– · –) ±15% relative error.

Beginning with case 1, $U_{mf,\text{expt}}$ reported by Franka et al. [3] is 19.9 cm/s and 7 correlations predict similar values within ±10%. The correlations that predicted acceptable values of $U_{mf}$ are based on Ref. [18, 23, 25, 30, 35, 36]. It is noteworthy that the modified Ergun equation [17], equation (7), performs very well when a granular material is relatively homogenous and can be represented by one characteristic particle diameter and density.

The experiments performed by Formisani [2] for the binary system (case 3) show that $U_{mf,\text{expt}} = 12$ cm/s. If we expand the error criterion to ±15%, then there are 3 correlations that perform well. The correlations that predicted acceptable values of $U_{mf}$ are based on Ref. [21, 24, 33]. The experiments related to the work by Jena et al. [4] for case 4 reported $U_{mf,\text{expt}} = 22.6$ cm/s. The correlation by Saxena & Vogel [24] predicts $U_{mf}$ within ±5% and 3 more correlations [17, 33, 38], predict values within ±15%.
Based on the study concluding section 5.1, it is clear that most correlations are system dependent and can not be readily used for an arbitrary system that is modeled with multiple components. However, if the granular material is relatively homogenous, many of the single-component correlations perform well (see Figure 5.6). The novel MASS method presented here seems to be an ideal way to estimate when a complex system of granular material will fluidize. Finally, we have demonstrated that the correlations by Saxena & Vogel [24] and Frantz [33] predicted $U_{mf}$ within $\pm 15\%$ relative error for multi-component systems. The following chapter will discuss how MFIX and the MASS method can be used to predict segregation for multi-component systems.
Chapter 6 Segregation in Multi-Component Systems

It was shown in Chapter 5 that the MASS method was able to predict fluidization behavior for multi-component systems. In addition, the MASS method provided information about the mass fractions of the unfluidized components, which can be used to predict the occurrence and extent of segregation for multi-component systems. The mass fractions of the unfluidized components can be compared to the inlet gas velocity to provide further information about segregation that the system may experience under the proper flow conditions. The mass fractions of an unfluidized and fluidized component can also be compared at a particular inlet gas velocity to determine mass fraction distribution throughout the domain.

6.1. Component Mass Fractions versus Inlet Gas Velocity

The MASS method uses mass fractions of each component that have not fluidized to determine pressure drop. The mass fraction relationship shown in Equation (75) can also be used to determine the extent of segregation that a system may experience. Both mass fraction $X_i$ and mass $m_i$ of each component can be calculated at each incremental inlet gas velocity to demonstrate how the bed changes during fluidization. Components do not fluidize at equal rates, therefore changes in $X_i$ or $m_i$ during fluidization can indicate the rate. It is important to note that when referring to the rate of fluidization of a component, this is a rate per inlet velocity (1/cm/s), not a rate per time (1/s). Therefore, the statement does not imply that at a given inlet velocity a component would fluidize more rapidly, but instead implies that at a given inlet velocity more/less of the initial mass of a component will be fluidized in comparison to another component at the same inlet velocity. The rate of change of $X_i$ and $m_i$ can be used to
qualitatively determine the extent of segregation that a system may experience given the proper flow conditions.

A visual tool to understand how $X_i$ changes for the unfluidized bed using different mixtures is shown in Figure 6.1. Figure 6.1 presents $X_i$ versus dimensionless velocity for four binary mixtures each with the same initial component mass fractions, $X_1 = 60\%$ and $X_2 = 40\%$, and component densities. The cases differ in the diameter difference between the system components $|D_1-D_2|$. As the gas velocity increases, the particles will not fluidize proportionally and can be tracked using Equation (75). Figure 6.1 shows how the two types of particles fluidize. As the gas velocity increases, $X_1$ increases because component 1 particles are more difficult to fluidize, while $X_2$ decreases because component 2 particles easily fluidize. Finally, at $U_g/U_{mf} = 1$, the entire bed fluidizes and $X_1 = X_2 = 0$. As components become more different ($|D_1-D_2|$ increases), the magnitudes of the initial slopes of the curves for $X_1$ and $X_2$ also increase. These trends can be used to qualitatively determine a system's propensity to segregate as demonstrated in the following examples.

![Figure 6.1 Influence of increasing $|D_1 - D_2|$ on component mass fractions versus dimensionless inlet velocity.](image)
To help understand the concept of using $X_i$ to predict segregation, consider case 2 from Chapter 5, which is a binary system with components that have the same density but different diameters ($D_1 = 499 \, \mu\text{m}$, $D_2 = 172 \, \mu\text{m}$). Initially the components have mass fractions of $X_1 = 25\%$ and $X_2 = 75\%$ in the unfluidized bed. Figure 6.2a shows how the two types of particles fluidize. As the gas velocity increase, $X_1$ increases because component 1 particles are more difficult to fluidize, while $X_2$ decreases because component 2 particles easily fluidize. Finally, at $U_g/U_{mf} = 1$, the entire bed fluidizes and $X_1 = X_2 = 0$. The behavior of case 2 does not show a high propensity for segregation, as the magnitudes of the initial slopes of the curves for $X_i$ and $X_2$ are small. Another way to consider fluidization is to examine the mass of the unfluidized material, $m_i$. As shown in Figure 6.2b, $m_2$ rapidly decreases with incremental increases in $U_g$ suggesting rapid fluidization of component 2. However, $m_1$ does not decrease as rapidly with incremental increases in $U_g$ suggesting a less rapid fluidization of component 1. Finally, at $U_g/U_{mf} = 1$, the entire bed fluidizes and $m_1 = m_2 = 0$.

Consider case 3 from chapter 5 which is a binary system like case 2 with the same component density but different diameters ($D_1 = 499 \, \mu\text{m}$, $D_2 = 271 \, \mu\text{m}$). Case 3 differs from case 2 because the second component diameter is larger in case 3 than in case 2. Initially the components have mass fractions of $X_1 = 25\%$ and $X_2 = 75\%$ in the unfluidized bed, which is the same as case 2. Figure 6.3 shows how the two types of particles fluidize. Case 3 demonstrates how components with a smaller diameter difference $|D_1 - D_2|$, will fluidize at a more even rate with increasing inlet velocity. The more even fluidization is shown by comparing Figure 6.2 and Figure 6.3, where the initial slopes of the curves for $X_i$ are smaller for case 3 than case 2, and the initial slopes of the curves for $m_1$ and $m_2$ are closer for case 3 than case 2. Therefore case 3 will produce less segregation than in case 2.
Figure 6.2 Glass beads, case 2 for (a) Unfluidized mass fraction versus dimensionless inlet gas velocity. (b) Unfluidized component masses versus dimensionless inlet gas velocity.

Figure 6.3 Glass beads, case 3 for (a) Unfluidized mass fraction versus dimensionless inlet gas velocity. (b) Unfluidized component masses versus dimensionless inlet gas velocity.

The effect of increasing difference in component densities $|\rho_1 - \rho_2|$ have been studied but are not presented here as they are similar to those findings for diameter differences. Figure 6.2 and Figure 6.3 can not predict the occurrence of segregation, but do provide insight into the potential for a fully fluidized system to segregate. The behavior of case 2 and 3 can be confirmed by
viewing the MFIX predictions for gas and solids volume fractions as shown in Figure 6.4 at $U_g/U_{mf} = 1.1$. Case 2 contours are shown in Figure 6.4(a-c) and case 3 contours are shown in Figure 6.4(d-f). It is apparent by comparing (a) and (d) that both cases are under similar flow conditions but case 2 has more gas flow through the center of the bed and is slightly more expanded. For both cases segregation between component 1 and 2 is shown with component 1 predominantly represented in the lower portion of the bed (frames b and e) and component 2 predominantly represented in the upper portion of the bed (frames c and f). Figure 6.4 confirms the previous predictions that case 2 and 3 do segregate after fluidization. Higher values of $U_g/U_{mf}$ will be presented later in Section 6.3.2 for a more segregated system.

To determine the occurrence of segregation, more information about the state of the unfluidized bed must be considered using the MASS method. The following section describes the procedure for predicting segregation in a fluidizing system.
Figure 6.4 Contours of volume fraction at $U_g/U_{mf} = 1.1$ for: case 2 (a) gas, (b) component 1, (c) component 2 and case 3 (d) gas, (e) component 1, (f) component 2.
6.2 Component Mass Fractions versus Dimensionless Bed Height

The MASS method can be used to predict the homogeneous unfluidized and fluidized mass fractions and the height of the unfluidized bed. By comparing the predicted mass fractions, \( X_i \), and the vertical height at any inlet gas velocity, it is possible to determine the occurrence of segregation during the fluidization process. The MASS method also provides the mass of each component, \( m_i \), present in the unfluidized bed at any gas velocity. The mass of each component can be used to solve for the height of the unfluidized portion of the bed by setting equation (2) equal to equation (3) and solving for \( h_0 \):

\[
h_0 = \frac{m}{\rho_b A} \quad (79)
\]

Substituting equation (4) into equation (79) and setting \( \varepsilon_s = (1 - \varepsilon_{mf,g}) \) results in:

\[
h_0 = \frac{m}{A \rho_s \left(1 - \varepsilon_{mf,g}\right)} \quad (80)
\]

As an approximation for the unfluidized bed height, the void fraction of the bed is assumed to remain constant until the entire bed is fluidized. Thus, it is possible to express the height of the unfluidized portion of the bed at any inlet gas velocity, \( k \), as:

\[
h_{unfluid}^k = \frac{\sum_{i=1}^{n} m_i^k}{A \left(1 - \varepsilon_{mf,g}\right)} \quad (81)
\]

The corresponding component mass fraction at a given gas velocity was shown in equation (75), where \( X_i^k = X_{i,unfluid}^k \), and represents the unfluidized bed component mass fractions, assuming the bed is homogeneous.

Using the fluidized component masses, \( A \Delta P_i^k/g \), and the total fluidized mass, \( A \Delta P^k/g \), it is possible to determine the fluidized mass fractions:
\[
X_{i,\text{fluid}}^k = \left( \frac{\frac{A \Delta P_i^k}{g}}{\frac{\Delta P_k^i}{g}} \right) = \frac{\Delta P_i^k}{\Delta P_k^i}
\]

(82)

One measure of segregation is the difference between the unfluidized component mass fraction and the fluidized component mass fraction \(|X_{\text{unfluid}} - X_{\text{fluid}}|\). A perfectly segregated bed would produce a value of unity, and smaller values represent less segregated systems. Another measure of segregation is when any region of the domain contains only one component, which is represented by a mass fraction of unity or zero in that region. These measures of segregation can be demonstrated by analyzing experimental cases presented in the next section.

6.3 Results and Discussion

6.3.1 Predicting Segregation Compared to Experiments

Formisani et al. [2] studied segregation in a binary mixture of glass beads using 2 characteristic particle diameters and recorded the distribution of the mass fraction of the smaller diameter particle at various inlet gas velocities. (Note: these cases are similar to those presented in Chapter 5) The conditions of the two cases studied by Formisani et al. [2] are shown in Table 6.1.

<table>
<thead>
<tr>
<th>Case</th>
<th>(m_1) (g)</th>
<th>(m_2) (g)</th>
<th>(\psi D_1) ((\mu m))</th>
<th>(\psi D_2) ((\mu m))</th>
<th>(\rho_1) (g/cm(^3))</th>
<th>(\rho_2) (g/cm(^3))</th>
<th>(\varepsilon_{g,mf})</th>
<th>(A_{c}) (cm(^2))</th>
<th>(U_{mf}) (cm/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>1615</td>
<td>538</td>
<td>499</td>
<td>172</td>
<td>2.53</td>
<td>2.53</td>
<td>0.336</td>
<td>80.12</td>
<td>12.3</td>
</tr>
<tr>
<td>11</td>
<td>1045</td>
<td>1045</td>
<td>499</td>
<td>271</td>
<td>2.53</td>
<td>2.53</td>
<td>0.375</td>
<td>80.12</td>
<td>14.2</td>
</tr>
</tbody>
</table>
Formisani et al. [2] experimentally measured mass fraction distributions by allowing a bed to reach quasi-steady state at a given inlet gas velocity and then instantaneously stopping the gas flow with a solenoid valve. The idea was to “freeze” the granular material in the state associated with that particular flow condition. The granular material was then vacuumed from the top of the stationary bed in horizontal layers with thicknesses of 1 cm – 2 cm. These layers where then sieved and weighed to determine the mass fraction of the small component, $X_{\text{small}}$, at the average sample vertical location, $Z$.

The experimental results for $Z$ versus $X_{\text{small}}$ for case 10 are shown in Figure 6.5(a-d) for inlet gas velocities of 1.4, 8.7, 9.7 and 13.4 cm/s. The initial mass fraction of the small diameter particle in the well-mixed bed is 0.25. The experiments show that with increasing $Z$, there is an increase in $X_{\text{small}}$. The MASS method is used to predict the $X_{\text{small, unfluid}}$ for the unfluidized bed, unfluidized bed height, $h_{\text{unfluid}}$, and fluidized component mass fraction, $X_{\text{small, fluid}}$, as discussed in Section 6.2. Figure 6.5a demonstrates how the MASS method predictions are applied to determine the $X_{\text{small}}$ distribution with vertical location. From the bottom of the domain ($Z = 0$ cm) to the unfluidized bed height ($Z = h_{\text{unfluid}}$) the domain is assumed to have a homogeneous mass fraction equal to $X_{\text{small, unfluid}}$. From the top of the unfluidized bed ($Z = h_{\text{unfluid}}$) to the top of the fluidized portion of the bed the domain is assumed to have a homogeneous mass fraction equal to $X_{\text{small, fluid}}$. In order to compare the experiments and MASS method, an average $X_{\text{small}}$ for the experiments was calculated using the trapezoidal rule, shown as a dotted line in Figure 6.5. The MASS method shows in Figure 6.5a that at an inlet gas velocity of 1.4 cm/s the smaller diameter particle is less present in the unfluidized bed and more present in the fluidized region with component mass fractions of 0.19 and 0.45, respectively. The resulting measure of segregation, $|X_{\text{unfluid}} - X_{\text{fluid}}| = 0.26$, shows a small amount of segregation at this inlet gas velocity.
A similar trend is also observed for the average experimental data where the unfluidized bed and fluidized region have component mass fractions of 0.18 and 0.55, respectively. At inlet gas velocities between 8.7 - 9.7 cm/s segregation is observed when $X_{small,unfluid} \approx 0$ (frames b and c). Here the mass fractions in the unfluidized bed are very close to zero, representing a region devoid of the smaller particle. At an inlet gas velocity of 13.4 cm/s, which is 1.1 $U_{mf}$, the entire bed is fluidized and becomes a homogeneous mixture. The resulting component mass fraction throughout the bed is very close to the original stationary system, $X_{small} = 0.25$. The results of the MASS method show good agreement with the experimental data.

The MASS method predictions for case 11 are also compared to the experimental data and averaged experimental data of Formisani et al. [2] as shown in Figure 6.6(a-d). The initial mass fraction of the small diameter particle in the well-mixed stationary bed is 0.5. Segregation is observed as inlet velocity is increased, however the same extent of segregation as observed in case 10 does not occur. $X_{small}$ in the unfluidized bed decreases from 50% to 10% (frames a to d) however it never reaches zero like in case 10. Likewise the height of the unfluidized portion of the bed decreases from $Z = 11$ cm to $Z = 0.6$ cm. The largest measure of segregation occurs at an inlet gas velocity of 15.2 cm/s and results in, $|X_{unfluidized} - X_{fluidized}| = 0.44$. These results are in good agreement with the experimental data.
Figure 6.5 Case 10 small diameter component mass fraction distribution with vertical height compared for experiments [2], averaged experiments, and new method for inlet gas velocities of (a) 1.4 cm/s, (b) 8.7 cm/s, (c) 9.7 cm/s and (d) 13.4 cm/s.
Figure 6.6 Case 11 small diameter component mass fraction distribution with vertical height compared for experiments [2], averaged experiments, and new method for inlet gas velocities of (a) $U_g = 3.1$ cm/s, (b) $U_g = 9.0$ cm/s, (c) $U_g = 13.2$ cm/s and (d) $U_g = 15.2$ cm/s.
Figure 6.7 Cases 10 and 11 unfluidized bed component mass fractions versus inlet gas velocity depicting propensity to segregate.

Case 11 demonstrates that smaller differences between particle diameters result in a lower tendency to segregate. The propensity to segregate for cases 10 and 11 can be analyzed using Figure 6.7 by observing the MASS method predicted unfluidized $X_i$ with dimensionless inlet velocity, as discussed in Section 6.1. The first observation from Figure 6.7 is that neither case shows a high propensity to segregate, which is determined by the small initial slopes of the curves. The second observation is that case 10 has a higher propensity to segregate, which is determined because $X_i$ approaches unity quicker. The qualitative observations from Figure 6.7 are in agreement with the findings shown in Figure 6.5 and Figure 6.6.

6.3.2 MASS Method Segregation Predictions Compared to MFIX Simulations

It was shown in Chapter 5 that MFIX predicted $\Delta P$ and $U_{mf}$ for binary and ternary systems. The simulations were found to be accurate within 7% average relative error of the experiments and the MASS method. Next, the MASS method will be compared to MFIX simulations to further examine segregation.
Revisiting case 3 discussed in Chapter 4 for Kaolin (Geldart B particle) and FCC (Geldart A particle), the MASS method is now used to predict the pressure drop curve. Figure 4.6c is repeated in Figure 6.8 for the experiments and MFIX data, and the MASS method predictions are added for comparison. The MASS method accurately predicts both the pressure drop and the minimum fluidization velocity for the binary system therefore, it is expected that the method can also predict segregation.

The unfluidized mass fraction trends with increasing inlet gas velocity as predicted by the MASS method are shown in Figure 6.9. The curves for Kaolin and FCC show a high propensity for segregation, illustrated by the large magnitude of the initial slopes of the curves. The case suggests that the larger, more slowly fluidizing Kaolin particle will dominate the lower region of the reactor, while the smaller, more quickly fluidizing FCC particle will dominate the upper region of the reactor.

Figure 6.8  Binary system of FCC and Kaolin pressure drop versus inlet gas velocity
The MASS method and MFIX simulations are used to demonstrate the $X_{FCC}$ distribution with height in Figure 6.10 for $U_g = 1, 4.3, 5.7, \text{ and } 6.5 \text{ cm/s}$. Heavy segregation can be seen in Figure 6.10 where at $U_g = 1 \text{ cm/s}$, the unfluidized bed is composed of 11% FCC, while the fluidized region is 60% FCC. This results in a predicted value of segregation of $|X_{FCC,\text{fluid}} - X_{FCC,\text{unfluid}}| = 0.49$. At higher inlet gas velocities, heavy segregation becomes more obvious when the unfluidized portion of the bed contains 0% FCC (only Kaolin is present). There is good agreement between the MFIX and MASS method for the prediction of segregation in the binary system.
It was shown that the binary mixture of Kaolin and FCC has a high propensity to segregate. Therefore it is expected that under the correct flow conditions, the system should demonstrate considerable segregation above the minimum fluidization velocity. MFIX simulations will be used to help visualize how the materials segregate.

Figure 6.11 and Figure 6.12 present volume fraction contours based on the MFIX simulations for $U_g = 7.2$ and $12.1$ cm/s, respectively. Shown are (a) gas, (b) Kaolin and (c) FCC volume fractions. The inlet gas velocity of $7.2$ cm/s is higher than the system minimum fluidization velocity of $6.8$ cm/s and within the bubbling flow regime. Figure 6.11a shows small gas bubbles (small “pockets” of red) that are indicative of a mildly bubbling bed. The volume fractions reveal that the region up to $4$ cm is dominated by the larger Kaolin particles (b), while the region from $4$ cm to $17$ cm is dominated by the smaller FCC particles (c). It is interesting to note that
the lower region and the upper region exhibit different flow characteristics. The upper region is clearly a bubbling flow regime, shown as the blue bubbles in Figure 6.11 (c), and the lower region demonstrates no bubbling behavior.

Figure 6.12 is data for \(U_g = 12.1 \text{ cm/s}\), which is a more rapidly bubbling bed. A small amount of segregation is observable with Kaolin slightly more prevalent in the lower region up to 9 cm (b), and FCC slightly more prevalent in the upper region from 9 cm to 19 cm (c). However, the extent of segregation is greatly reduced and the Kaolin and FCC particles are fluidizing to create a relatively well-mixed bed.

Previous research has suggested that the amount of segregation after fluidization is determined by the flow regime of the mixture [6]. However, from the findings presented here it seems likely that differing component flow regimes promote high segregation while similar component flow regimes promote less segregation. At an inlet gas velocity of 7.2 cm/s the FCC is well above its individual component minimum fluidization velocity of 0.2 cm/s and exhibits a bubbling flow, while the Kaolin is just slightly above its individual component minimum fluidization velocity of 6.8 cm/s and experiences no bubbling behavior. The difference between the FCC and Kaolin flow regimes promotes heavy segregation between the components. At an inlet gas velocity of 12.1 cm/s the FCC exhibits a heavy bubbling flow and Kaolin exhibits a bubbling flow. The similarity between the FCC and Kaolin flow regimes promotes mixing between the components. Similarly, the heavy segregation experienced at inlet gas velocities bellow the systems minimum fluidization velocity is the result of dissimilar component flow regimes. An example is at \(U_g = 4.3 \text{ cm/s}\), which is below the minimum fluidization velocity of Kaolin, \(U_{mf,Kaolin} = 6.8 \text{ cm/s}\), and above that of FCC, \(U_{mf,FCC} = 0.2 \text{ cm/s}\). Therefore the FCC is in
the fluidized flow regime and the Kaolin is not, resulting in heavy segregation between the components in the bed as shown in Figure 6.10.

Figure 6.11 Binary system instantaneous volume fraction MFIX simulations for inlet velocity of 7.2 cm/s (a) gas, (b) Kaolin, and (c) FCC

Figure 6.12 Binary system instantaneous volume fraction MFIX simulations for inlet velocity of 12.1 cm/s (a) gas, (b) Kaolin, and (c) FCC
Chapter 7 Conclusions

The work presented in this thesis focused on advancing current knowledge on multi-component fluidization through the use of numerical and predictive techniques. MFIX simulations were used to study a two-stage reactor geometry with a binary mixture of Kaolin and FCC. It was shown that MFIX can accurately predict pressure drop versus inlet gas velocity for binary mixtures. The MFIX simulations also demonstrated how inlet gas velocity influences bed segregation in two-stage reactors. MFIX was shown to be a valuable tool in predicting and designing fluidized beds.

A new method was developed to predict the pressure drop versus inlet gas velocity and minimum fluidization velocity for multi-component fluidized beds. The method accounts for the changing bed composition during the fluidization process by using a novel definition for the mass fractions of the bed not yet fluidized. Published experimental data for pressure drop from single-, binary- and ternary-component fluidized bed systems were compared to MFIX simulations and the MASS method, with good agreement between all three approaches. Minimum fluidization velocities predicted using correlations in the literature were compared with the experimental data, MFIX, and the MASS method. The predicted minimum fluidization velocity from the MASS method provided very good results with an average relative error of ±4%. The MASS method was shown to accurately predict when complex multi-component systems of granular material will fluidize.

The MASS method and MFIX were also used to explore the occurrence and extent of segregation in multi-component systems. It was demonstrated that the MASS method predicted unfluidized mass fractions as a function of inlet velocity to predict the propensity for a mixture to segregate. It was also demonstrated that the MASS method could predict average particle
distributions throughout the reactor domain. The results were compared to both experimental data and MFIX simulations with good agreement. Therefore, it is concluded that the MASS method and MFIX can accurately predict the occurrence and extent of segregation a system may experience.

In summary, MFIX and the MASS method can both be used to appropriately model and predict the behavior of bubbling fluidized beds. These methods are capable of aiding in the design, operation and study of bubbling fluidized beds.
Bibliography


