Bubble Dynamics in a Sand Fluidized Bed in the Presence of Biomass Pellets

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A thesis submitted in partial fulfillment of the requirements for the Doctor of Philosophy degree in Chemical and Biochemical Engineering

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Abstract

Given the worldwide concerns regarding fossil fuel availability, global warming, water, and air pollution and economy needs, there is an urgent requirement to develop and implement alternative energies. Biomass gasification can consume vegetal waste to produce syngas, which is a mix of carbon monoxide, hydrogen, and carbon dioxide. When biomass gasification is carried out in a fluidized bed, the process is highly efficient.

The experimental study of the present Ph.D. dissertation took place in a Plexiglas 0.44 m diameter unit, equipped with a CREC Optiprobe system and a video camera. The unit was filled with 200-900 µm sand particles and biomass pellets measuring 2.7 cm in length and 0.8 cm in diameter. This was used to take experimental measurements of bubbles size, velocity, and shape.

Single bubbles injected in a sand bed at minimum fluidization with and without biomass were first considered. Later, bubbles evolving in a sand bed, operating in the dense phase bubble regime were studied. On this basis, the capabilities of a developed geometrical model to predict the BAC (Bubble Axial Chord) and the BACs correlated with the BRVs (Bubble Rising Velocity) were examined. The bubble dynamics model considered includes an adjustable bubble wake parameter, with predictions providing the bubble chord, the bubble frontal-radius, and the bubble rising velocity. Following this step, the effects of biomass pellet addition on the BAC, the BRV, and the bubble assigned shape were evaluated.

Computational Fluid Dynamics Multiphase Particle-in-Cell (CFD-MPPIC) simulation using a CPFD Barracuda VR® v17.4.1 software was considered, and this for the various cases studied. The proposed CFD-MPPIC model involved the following: a) an equivalent 1 cm³ biomass pellets, b) an adjusted particle drag model, c) a bubble-wall interaction, d) a selection of
computational cells, e) a Multiphase Particle-in-Cell population sizing, and f) a cell distribution implemented throughout the column.

Experimental results in the Plexiglas 0.44 m diameter unit, validated the proposed CFD-MPPIC model with good predictions of both BACs and BRVs. This was the case for all conditions studied, with the only exception of bubbling beds with added biomass, where calculated BRVs were found for some operating conditions as less trustable.

**KEYWORDS:** Gasification, Computational Fluid Dynamics, Multiphase Particle-in-Cell, CFD-MPPIC, Gasification, Fluidized Bed, Single Bubble, Biomass.
Lay Abstract

The world urgently needs to address pollution, fuel depletion, and energy accessibility using innovative ways to transform energy resources. Biomass is present in every plant dead or alive in many locations around the world and can be used as a source of renewable energy. Agricultural waste, for example, is an issue for most farmers since it increases the cost of production, given its disposal fees.

Biomass gasification in fluidized beds is a technology that can help to mitigate agricultural waste toxicity. It can convert it into synthesis gas (syngas), which is a valuable product that can be used to produce chemicals or be employed as a fuel due to its heating value.

Typically for biomass gasification in a fluidized bed, a combined flow of air and stream is circulated upwards in the form of bubbles. This contributes to both gasification and sand mixing, with gasification taking place at a close to a constant temperature.

Designing, scaling-up, and operating these units can be facilitated by using fiber optic sensors as well as by performing numerical calculations based on fundamental physicochemical principles. Using this approach, the present Ph.D. dissertation studies bubble dynamics in a sand fluidized bed prototype with and without biomass pellets. On this basis, both the size and velocity of the formed bubbles are measured experimentally and predicted with the proposed mathematical model.

As a result, the outcome of this project provides a better understanding of bubble phenomena in sand fluidized bed gasifiers, as well as contributes to the establishment of numerical tools for designing, predicting, and controlling the operation of this kind of unit.
Dedicated to Hera and Fernando. Because everything I do, I do because of them.

They are my greatest achievement in life.

Dedicado a Hera y Fernando. Porque todo lo que hago, lo hago por ellos.

Son el mayor logro de mi vida
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“If I have seen further it is by standing on the shoulders of Giants.”

-Sir Isaac Newton

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## Nomenclature

### Symbols

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<th>Symbol</th>
<th>Unit</th>
<th>Description</th>
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<tr>
<td>(A)</td>
<td>(\text{m/s}^2)</td>
<td>Discrete Particle Acceleration</td>
</tr>
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<td>(A_r)</td>
<td>-</td>
<td>Archimedes Number</td>
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<td>(c_1, c_2, c_3)</td>
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<td>(C_d)</td>
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<td>Drag Coefficient</td>
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<tr>
<td>(D_{\text{bed}})</td>
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<td>(d_{\text{beq}})</td>
<td>(\text{m})</td>
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<td>(D_p)</td>
<td>(\text{N})</td>
<td>Particle Drag Force</td>
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<tr>
<td>(F)</td>
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<td>Rate of Momentum Exchange per Volume Between the Fluid and the Particles</td>
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<td>Standard Acceleration due to Gravity (9.8 m/s²)</td>
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</tr>
<tr>
<td>(V_T)</td>
<td>(\text{m}^3)</td>
<td>The volume of the Sphere Containing the Gas and the Wake</td>
</tr>
<tr>
<td>(V_w)</td>
<td>(\text{m}^3)</td>
<td>The volume of the Wake Portion of the Sphere</td>
</tr>
<tr>
<td>(V_{rp})</td>
<td>(\text{m/s})</td>
<td>Terminal Velocity</td>
</tr>
<tr>
<td>(x, y)</td>
<td>(\text{m})</td>
<td>Cartesian Coordinates</td>
</tr>
</tbody>
</table>
### Greek Symbols

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha$</td>
<td>Angle Between the Center of the Circumference and the two minimums of the double parabola function</td>
</tr>
<tr>
<td>$\beta, \epsilon$</td>
<td>Dimensionless Adjustment Parameters Used for the Particle Stress Calculation</td>
</tr>
<tr>
<td>$\theta_{CP}$</td>
<td>Dimensionless Close-Packed Particle Volume Fraction</td>
</tr>
<tr>
<td>$\theta_f$</td>
<td>Dimensionless Fluid Volumetric Fraction</td>
</tr>
<tr>
<td>$\theta_p$</td>
<td>Dimensionless Particle Volumetric Fraction</td>
</tr>
<tr>
<td>$\theta_w$</td>
<td>Dimensionless Wake Angle</td>
</tr>
<tr>
<td>$\mu_s$</td>
<td>${ Pa \cdot s }$ Shear Viscosity</td>
</tr>
<tr>
<td>$\rho_f$</td>
<td>${ kg/m^3 }$ Fluid Density</td>
</tr>
<tr>
<td>$\rho_p$</td>
<td>${ kg/m^3 }$ Particle Density</td>
</tr>
<tr>
<td>$\sigma_s$</td>
<td>${ V }$ Standard Deviation of the Voltage Data Series</td>
</tr>
<tr>
<td>$\tau_f$</td>
<td>${ Pa }$ Non-hydrostatic component of the stress</td>
</tr>
<tr>
<td>$\phi$</td>
<td>Dimensionless Particle Probability Distribution Function</td>
</tr>
<tr>
<td>$\psi$</td>
<td>Dimensionless Particle Sphericity</td>
</tr>
</tbody>
</table>

### Acronyms

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>BAC</td>
<td>Bubble Axial Chord</td>
</tr>
<tr>
<td>BIAS</td>
<td>Mean Signed Error</td>
</tr>
<tr>
<td>BLM</td>
<td>Baseline Multiplicator</td>
</tr>
<tr>
<td>BM</td>
<td>Biomass</td>
</tr>
<tr>
<td>BM vol%</td>
<td>Volume Percentage of Biomass Content in the Bed</td>
</tr>
<tr>
<td>BRV</td>
<td>Bubble Rise Velocity</td>
</tr>
<tr>
<td>CFD</td>
<td>Computational Fluid Dynamics</td>
</tr>
<tr>
<td>CREC</td>
<td>Chemical Reaction Engineering Center</td>
</tr>
<tr>
<td>DEM</td>
<td>Discrete Element Method</td>
</tr>
<tr>
<td>FR</td>
<td>Bubble Frontal Radius</td>
</tr>
<tr>
<td>HESC</td>
<td>Hybrid Experiment-Spherical Cap</td>
</tr>
<tr>
<td>MRAE</td>
<td>Mean Relative Absolute Error</td>
</tr>
<tr>
<td>MRSE</td>
<td>Mean Relative Signed Error</td>
</tr>
<tr>
<td>NOBM</td>
<td>No biomass added (0 % biomass)</td>
</tr>
<tr>
<td>MPPIC</td>
<td>Multiphase Particle in Cell</td>
</tr>
<tr>
<td>PSD</td>
<td>Particle Size Distribution</td>
</tr>
<tr>
<td>NNTBAC</td>
<td>Non-Treated Bubble Axial Chord</td>
</tr>
<tr>
<td>RMSE</td>
<td>Root Mean Squared Error</td>
</tr>
<tr>
<td>SE</td>
<td>Standard Error</td>
</tr>
<tr>
<td>Syngas</td>
<td>Synthesis Gas</td>
</tr>
<tr>
<td>TFM</td>
<td>Two Fluids Model</td>
</tr>
<tr>
<td>vol%</td>
<td>Volume percentage</td>
</tr>
</tbody>
</table>
Chapter 1: Introduction

The earth’s fossil fuels cannot be considered an endless energy resource. (Höök and Tang, 2013; Shafiee and Topal, 2009). Global warming and air pollution cause health issues and have, as a result, associated economic costs (Hansen et al., 2006; Vermeer and Rahmstorf, 2009). While there is an ongoing debate about the anthropogenicity of CO₂ emissions (Cook et al., 2013; Tol, 2014), urgent action is needed to alleviate the negative impact of CO₂ emissions. It is thus, anticipated that a sensible way to improve future world population health and the global economy is to modify how energy is produced, as well as how goods and services are obtained. Given this scenario, science and engineering researchers are engaged in the development and implementation of alternative energy production (Foley et al., 2015).

When alternative energy technologies are reviewed, one can notice that the harvesting of solar, wind, and tidal sources are strongly dependent on location, weather, and seasons (Lakatos et al., 2011). Nuclear power, on the other hand, has the intrinsic risk of dangerous nuclear accidents. Thus, biomass conversion appears to be a potentially more reliable alternative energy source, less dependent on weather, seasons, and locations.

Biomass was the first fuel to be used by humans in prehistorical times (Bithas and Kalimeris, 2016), and this is given its combustibility. One of the advantages of biomass resides in biomass ability to help produce a steady power production. This is in contrast with the variability of energy production when all the other types of alternative technologies are used. Biomass production mainly depends on the capacity of gathering and processing biomass. The National Renewable Energy Laboratory (Nrel Laboratory, 2006) estimates that it is possible to reduce 30%
of petroleum usage in the United States, if 1.3 billion tons of biomass were produced, and used to manufacture fuels.

On top of that, biomass can be used to manufacture chemical products capable of substituting hydrocarbon-based products (Boerrigter and Rauch, 2006; Johansson, 2016). Thus, biomass conversion can play a significant role in the future of energy production. However, this is with the condition that several pending issues are addressed (Berndes et al., 2003).

There are different ways to transform biomass into power. The conventional and simplest approach, although not the most adequate, is to burn biomass. This is inefficient as it creates contaminants, and as a result, is not a recommended alternative. Furthermore, there are other methods to transform biomass into gas or liquid fuels. These approaches involve chemical or biochemical processes as well as other options like biogas digestion (Balat and Balat, 2009) or gasification (Göransson et al., 2011). These two techniques have something in common; they both use biomass as the raw material to produce fuel in a gaseous form. While bio digestion is meant to produce biogas, gasification aims to make producer gas or synthesis gas. Any of these gases can be burned in a combustion engine or used to generate electrical power through a fuel cell (Wender, 1996).

1.1 Biomass

Biomass is any organic matter that is derived from plants or animals. Its chemical composition is variable, depending on its origin and previous treatments. In general terms, its basic components are primarily carbon, hydrogen, and oxygen. Other valuable mineral elements are present; however, in lesser quantities (de Lasa et al., 2011).
Due to its components, biomass can be used to produce either biogas or syngas by utilizing different processes. There are important differences between these two gases, basically in their methane and hydrogen contents. While biogas has a methane content between 55% and 65%, syngas barely has a 0% to 5 of methane. This is important to note, due to the known methane potential as a greenhouse gas (Solomon et al., 2007). Furthermore, while syngas has a hydrogen content of between 25% to 30%, biogas has a hydrogen content between 0% and 1%. Typical compositions of these two gases are reported in detail in Table 1-1 (Balat and Balat, 2009; National Energy Technology Laboratory, 2015).

Biodigestion has a retention time of between 30 and 60 days and is a process that is carried out at temperatures between 25°C and 60°C (Balat and Balat, 2009). Gasification, on the other hand, takes minutes to occur, requiring, however, higher temperatures between 650°C and 1200°C.

<table>
<thead>
<tr>
<th>Biogas Components</th>
<th>Syngas Components</th>
</tr>
</thead>
<tbody>
<tr>
<td>Component</td>
<td>Quantity (%)</td>
</tr>
<tr>
<td>Methane (CH4)</td>
<td>55 - 65</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>35 - 45</td>
</tr>
<tr>
<td>Hydrogen Sulfide (H2S)</td>
<td>0 - 1</td>
</tr>
<tr>
<td>Nitrogen (N2)</td>
<td>0 - 3</td>
</tr>
<tr>
<td>Hydrogen (H2)</td>
<td>0 - 1</td>
</tr>
<tr>
<td>Oxygen (O2)</td>
<td>0 - 2</td>
</tr>
<tr>
<td>Ammonia (NH3)</td>
<td>0 - 1</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Biomass mainly from vegetal origins is used in gasification. This is the case given its limited water content. On the other hand, other available sources such as animal waste contain too much water and, as a result, are normally excluded as gasification feedstocks. This is the case given too much energy has to be spent to vaporize water bringing the entire feedstock to the desired thermal gasification levels.
There are differences in biomasses depending on their sources. We can mainly distinguish four principal categories due to their original purposes (de Lasa et al., 2011):

(i) *Energy Crops.* These are grown to be a biomass source. However, from all the possible biomass sources, this is the least recommended one since it entails a change of soil use normally employed for food crops. The use of this kind of biomass source can also cause economic problems since prices for food crops could rise, supply shortages in the food industry (Martin, 2010).

(ii) *Agricultural residues and waste.* This category refers to the fraction of the agricultural product that cannot be consumed for different reasons (e.g., imperfection or disease in the plant). This category is the closest to being carbon neutral since it uses an already available agricultural waste. As a result, its use does not inflict ecological damage. Furthermore, in some cases, as in the case of Costa Rica coffee production, it can address a major environmental issue in the disposal of the coffee broza (coffee waste) (Torres et al., 2016).

(iii) *Forest waste and residues.* They consist of all the wood, leaves, branches, and roots, in general, organic material that is no longer attached to a tree or plant in a forest.

(iv) Industrial and municipal wastes. This category includes municipal solid waste, sewage sludge, and industrial waste, mainly from the paper industry.

The European Bioeconomy Network (EUBIONET) (Alakangas, 2006) classifies biomass by its content into four categories: (i) woody biomass, (ii) herbaceous biomass, (iii) fruit biomass and (iv) blends and mixtures.

The estimated total biomass production in the world in 1998 was 104.9 petagrams of carbon per year (Field C B et al., 1998). According to Hoogwijk et al., (Hoogwijk et al., 2003), biomass energy has the potential to become a worldwide alternative to fossil fuels, as long as the public
policies allow it, even if its carbon neutrality is questioned by some (Johnson, 2009; Zanchi et al., 2012).

While considering biomass to produce energy and valuable chemicals, one should act with caution. For instance, using biomass from agricultural waste may have a negative impact on the soil, given that the soil may be progressively deprived of valuable nutrients (Huber et al., 2006). In order to ease this undesirable effect, incomplete waste gasification with biochar production, which is a valuable solid residue containing most of the biomass mineral matter, is recommended (Torres et al., 2019).

In other cases, however, removing biomass from the soil can have a positive environmental impact. This is the case of the removal of broza in Costa Rica. Broza is the waste left from coffee harvesting. If left in the soil, it ferments, releasing both methane, a high impact greenhouse gas, and other toxic chemical species. Thus, broza gasification is beneficial to provide a sustainable approach to coffee production. Therefore, the proper use of biomass as a feedstock to produce valuable goods may offer a two-way solution, providing alternative energy as well as preserving the nutrients and healthy conditions of agricultural lands.

1.1 Gasification

In order to transform biomass into some form of energy, there are several options at hand. Most commonly, the conversion can be thermal, chemical, biochemical, or electrochemical. The thermal options are combustion, torrefaction, pyrolysis, and gasification. The main difference between these four processes is the amount of oxygen required and the temperature used. Details of this are provided in Table 1-2.
Table 1-2. Difference Between Thermal Processes.

<table>
<thead>
<tr>
<th>Thermal processes (Biomass)</th>
<th>Process</th>
<th>Oxidizer (Oxygen)</th>
<th>Temperature</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Torrefaction</td>
<td>0%</td>
<td>200 – 300 °C</td>
</tr>
<tr>
<td></td>
<td>Pyrolysis</td>
<td>0%</td>
<td>300 – 650 °C</td>
</tr>
<tr>
<td></td>
<td>Gasification</td>
<td>&lt;100%</td>
<td>&gt;700 °C</td>
</tr>
<tr>
<td></td>
<td>Combustion</td>
<td>≥100%</td>
<td>230 °C</td>
</tr>
</tbody>
</table>

The main benefit of using gasification resides in the generated product. A syngas with limited tar content is produced from the gasification of biomass. This syngas can be purified removing CO₂, sulfur and nitrous oxides, as well as trace amounts of contaminants such as mercury, arsenic, selenium, cadmium. Process temperatures and pressures facilitate syngas post-processing without additional energy requirements. Another advantage of biomass gasification resides in the flexibility of gasifiers, given that they can be fed several types of feedstocks ranging from coal to biomass.

Gasification is a thermal process that converts organic or fossil fuels based on a carbonaceous material into syngas by exposing them to high temperatures (>700°C) under a limited oxygen atmosphere. Along with synthesis gas production, some liquid and solid hydrocarbons are generated. Tars are considered harmful to the gasification process since they have multiple negative influences on the reactor’s behavior and the produced syngas quality (Han and Kim, 2008).

While gasification is not a new technology, it still requires major improvements. The process is known since the 1800s, but its use was replaced by natural gas and electricity during the industrial revolution. Nevertheless, in the 1920s, it played a significant role in the production of synthetic chemicals. Furthermore, during the 1940s, automobiles were built based on being fueled by “wood gas.” The syngas provided was directly in a built-in automobile gasifier.
Inside a gasifier, the biomass undergoes several physical-chemical transformations. Dehydration occurs at the beginning, at a temperature around 100° up to 200°C. This reduces the weight of the biomass up to 40%. After the dehydration, the torrefaction and pyrolysis (or devolatilization) occur between 200 and 650 °C. During this process, more weight is lost, resulting in a total of 70% of the mass decrease. Finally, this is followed by the gasification stage, where the final conversion happens, and the syngas is produced.

The gasification mechanism aims to break down hydrocarbons into low molecular weight gases through the following processes: First, the biomass is thermally depolymerized. This is followed by reforming and partial combustion reactions. The principal heterogeneous and homogeneous steps, including drying, pyrolysis, char gasification, reforming, and partial and complete oxidation, are summarized in Table 1-3.

There are multiple types of gasifiers. All of them have different characteristics. They can be categorized into three types: fixed bed, fluidized bed, and entrained bed. Only the first two types are used in biomass gasification (de Lasa et al., 2011).

Fixed bed gasifiers can be of the downstream, upstream, and crossflow type. All fixed bed gasifiers contain reduction-oxidation zones. However, these zones may be placed in different orders accordingly to the configurations. Drying, pyrolysis, reduction, and combustion zones are described in Figure 1-1 for the three types of fixed bed gasifiers.
### Table 1-3. Main Gasification Reactions (Dai et al., 2015).

<table>
<thead>
<tr>
<th>Reaction Name</th>
<th>Reaction Formula</th>
<th>$\Delta H_{298K, 1atm}$ (kJ/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Heterogeneous Reactions</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Water-Gas – Primary</td>
<td>$C(s) + H_2O \rightleftharpoons CO + H_2$</td>
<td>131.3</td>
</tr>
<tr>
<td>Water-Gas – Primary</td>
<td>$C(s) + 2H_2O \rightleftharpoons CO_2 + 2H_2$</td>
<td>90.2</td>
</tr>
<tr>
<td>Boudouard Reaction</td>
<td>$C(s) + CO_2 \rightleftharpoons 2CO$</td>
<td>172.4</td>
</tr>
<tr>
<td>Oxidation</td>
<td>$C(s) + O_2 \rightarrow CO_2$</td>
<td>-392.5</td>
</tr>
<tr>
<td>Partial Oxidation</td>
<td>$C(s) + 1/2 O_2 \rightarrow CO$</td>
<td>-110.5</td>
</tr>
<tr>
<td>Methanation</td>
<td>$C(s) + 2H_2 \rightarrow CH_4$</td>
<td>-74.6</td>
</tr>
<tr>
<td><strong>Homogeneous Reactions</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Water-Gas-Shift</td>
<td>$CO + H_2O \rightleftharpoons CO_2 + H_2$</td>
<td>-41</td>
</tr>
<tr>
<td>$H_2$/(Steam) Reforming</td>
<td>$CO + 3H_2 \rightleftharpoons CH_4 + H_2O$</td>
<td>(-/+ 205.9)</td>
</tr>
<tr>
<td>Oxidation Reactions</td>
<td>$CO + 1/2 O_2 \rightarrow CO_2$</td>
<td>-283</td>
</tr>
<tr>
<td></td>
<td>$H_2 + 1/2O_2 \rightarrow H_2O$</td>
<td>-242</td>
</tr>
<tr>
<td>Steam Reforming</td>
<td>$CH_4 + 2H_2O \rightleftharpoons CO_2 + 4H_4$</td>
<td>164.7</td>
</tr>
<tr>
<td>$CO_2$ Reforming</td>
<td>$C_6H_6O + 5H_2O \rightarrow 6CO + 8H_2$</td>
<td>642</td>
</tr>
<tr>
<td></td>
<td>$CH_4 + CO_2 \rightleftharpoons 2CO + 2H_2$</td>
<td>247</td>
</tr>
</tbody>
</table>

![Figure 1-1. Different Types of Fixed Bed Gasifiers (Lindström, 2006).](image-url)
Fluidized bed gasifiers use a fine granular material (e.g., sand) as a medium to perform the gasification. This fine granular material is mixed with gas (e.g., air) and made to behave like a fluid. Due to this fluidization, the medium has a homogeneous temperature and excellent mixing properties, in addition to a lower tar content compared to the medium of the fixed bed gasifiers (de Lasa et al., 2011).

This type of reactor can be classified into two types: circulating and bubbling. In the first type, the biomass and sand mix is circulated through the gasifier and a cyclone, being returned continuously through the unit dip leg, as in Figure 1-2. The second kind of gasifier consists of a vessel with a perforated bottom that can be used to push air through the bed, causing fluidization. In this type of reactor, all the reaction steps that usually take place in gasification occur. Due to the mixing of the bed, however, there are no discernible zones like those in the fixed bed reactor.

In 2008, Wang et al. (Wang et al., 2008) summarized the advantages and technical challenges of each kind of gasifier and each parameter involved in the gasification process.
1.2 Fluidization

Fluidization is a process where a gas (e.g., air) is forced to flow through a bed containing a solid sand-like material making it behave like a fluid. In his patent, Winkler in 1928 described the process as:

“...consists in charging the small coal material onto a suitable grate or support in a shaft generator, and blowing a gasifying medium, such as air or air and steam through the said coal material either alternately or jointly according to the kind of fuel gas desired with sufficient pressure to bring about a strong agitation in the form of a so-to-say boiling motion of the material.” (Winkler, 1928)

Particles become fluidized when an upward flowing gas imposes a high enough drag force to overcome the downward force of gravity (Cocco et al., 2014). This implies that the velocity at which gas enters the bed affects the extent of particle fluidization. This is the case because the velocity of the gas is directly related to the amount of frictional drag force that the gas imposes on the material.

When the gas starts to be pumped into the bed, there is a gas pressure drop in the bed. This is caused by the kinetic energy loss, which is transferred from the gas to the particles. Research has been done regarding the effect of the velocity on gas pressure drop in the bed. It has been demonstrated that while the velocity of the gases increases, the pressure drop also increases. The height of the bed remains the same until it reaches the so-called minimum fluidization velocity. Following this, while the velocity of the gas further augments, the bed height increases until it reach a maximum value, with the gas pressure drop remaining close to constant, as shown in Figure 1-3.
In 1966, Wen and Yu (Wen and Yu, 1966) developed a model that relates the Reynolds number (Re) to the Archimedes number (Ar). This enabled researchers to calculate the minimum fluidization velocity. In the same way, the fluidization height could be related to the pressure drop through the density of the bed, the rate of the gravity, and the force-weight conversion factor (Cocco et al., 2014). Some efforts had been made to improve the Wen and Yu model, as for example, in the work of Delebarre in 2004 (Delebarre, 2004). However, the original model by Wen and Yu is still the most commonly used.

Once the minimum fluidization velocity has been reached, if the gas velocity keeps increasing, bubbles form, and the dynamics of the particles in the bed change (Figure 1-3), therefore, the reactor should then be treated like a two-phase system where a bubble phase and a dense phase interact. The more the velocity of the gas increases, the bigger the size of bubbles in the bed. Describing bubble formation and bubble dynamics is important because mass transfer between the two phases is a critical feature in the interphase interaction and, as a result, reactor modeling.
Figure 1-4. Effect of the Gas Velocity in the Bed Hydrodynamics (Cocco et al., 2014).

Nevertheless, fluidization velocity is not the only parameter that influences bubble development. The size of the particles also plays a big role in this matter.

In the 1970s, Geldart (Geldart, 1973, 1972) predicted that the behavior of the phases is strongly influenced by particle size and density of the sand-like medium. They divided particles into 4 groups, as shown in Figure 1-5.

Figure 1-5. Geldart Particles Classification (Geldart, 1973).
Particles on the group A fluidize well. They do not promote the formation of big bubbles. As a result, this moderates bubble velocity and improves mass transfer between phases. Group B particles tend to have more violent fluidizations as their minimum fluidization velocity, and their minimum bubbling velocity is almost the same. Fluidization beds formed with Group B particles tend to produce bigger bubbles faster with a decrement of the mass transfer between phases. Type C particles are the most difficult to fluidize. Due to their cohesiveness, Type C particles experience channeling (preferential flow). Finally, type D particles are the biggest among all. Their higher gas velocity requirements to reach fluidization result in turbulent behavior.

The rate of heat and mass transfer processes, as well as the reaction rate in a fluidized bed gasifier, depend on the interaction of the gas and solids within the bed (Kunii and Levenspiel, 1991). A phenomenological model to represent the flow of gases through the bed is necessary to provide a better understanding and description of the internal processes. Any fluidized bed will have zones of low solid density called bubbles or voids. Bubbles transport the fluid throughout the bed. These bubbles, therefore, are an important part of the gasification process in a fluidized bed, since they are the most significant factor in the mixing and transfer phenomena inside the bed.

Due to their potential value for biomass gasification, dense phase fluidized bed gasifiers must be studied. Although experimental data is possible to obtain, there are limitations on what can be measured, and the building cost of the models commonly impede progress. Computational Fluid Dynamics is an alternative to solve this problem since it allows one to study the behavior of the reactor under a range of operational conditions without elevating the reactor fabrication cost.

Regarding Computational Fluid Dynamics (CFD), these models of fluidized must be validated with experimental data. This means that until this test is not passed, the CFD model cannot be considered for unit up-scaling or for analyzing operational condition changes. The
The easiest way to approach CFD validation is to retain the variables that could have a significant effect and to systematically change them until one obtains values near to experimental data. Following this, one can increase the number of other variables until one accurately reproduces experiment data. For instance, one possible approach is to use a single bubble to produce a bubble absent from wall effects and one which depends on particle drag and particle collision only.

Chapter 2 of this thesis will introduce the bibliographic review from which the mathematical models and correlations used during this study are taken. Chapter 3 will present the objectives of the study as well as the research achievements. Chapter 4, based on our published paper (Torres Brauer et al., 2020), explores the mathematical modeling developed for this study, in order to interpret the experimental data of a single bubble measurement. Chapter 5 will explain the novelty of the developed methodology used to find the baseline of the data series and utilized to establish the treatment required to translate the CREC Optiprobe voltage data into bubble size and velocity.

Chapter 6 introduces the challenges that the data analysis of the CREC Optiprobe system represents and how they were approached. Chapter 7 discusses the experimental results with the use of the described data analysis.

Chapter 8 will report in detail the procedure followed to produce a simulation of the single bubble exercise, from the grid to the drag model selection. Chapter 9 presents the numerical results and their respective discussion.

Chapter 10 explores the operation of the reactor under a constant flow of air through the distributor and how the experimental measurements compare with the ones obtained numerically.
1.3 Conclusions

There are different ways in which the gasification of biomass can be achieved. In this research, we use a fluidized bed reactor gasifier. In the fluidized bed, high rates of mass and heat transfer are achieved, and this is obtained with a near-zero temperature gradient (de Lasa et al., 2011).

The objective of this Ph.D. study is to provide a better understanding of the fluid dynamic phenomena that drive the operation of the fluidized bed gasifier, allowing the transformation of biomass into syngas. By using our experimental results and relying on the numerical simulation, we attempt to gain awareness of the bubble behavior and the effects of the operational conditions over the bubble physics. Regarding the CFD simulation, there are many factors that may affect the hydrodynamics of the sand particles in a fluidized bed. Gas velocity, particle size, pressure drop, bed height, bubble size, and velocity and bed geometry are some of the most important parameters that should be measured in order to understand the inner physics in a fluidized bed.
Chapter 2: Bibliographic Review

Extensive research has been developed on single bubbles in beds of Group A powders in the Geldart classification (Karimipour and Pugsley, 2011; Kunii and Levenspiel, 1991; Mori and Wen, 1975). Studies with Group B powders in the Geldart classification with densities in the 2000-3000 kg/m$^3$ range are, however, less frequent, including their interaction with larger bodies such as bubble breakers often called internals. When internals are added to a fluidized bed, the bubbles change their behavior (Bhusare et al., 2017; Dutta and Suciu, 1992; Ramamoorthy and Subramanian, 1981; Van Dijk et al., 1998) by breaking more often and therefore, leading to smaller bubble sizes. As the bubbles become smaller with the addition of biomass, they multiply in number, and the contact area between the bubbles and the dense phase increases significantly, greatly helping the mass chemical species exchange between the two phases.

However, and given the value of fluidized beds for biomass gasification, additional research is required using Geldart type B powders, particularly of those of higher densities ($\rho\geq2500$ kg/m$^3$), including fluidized sand beds loaded with biomass pellets. There are, in this respect, few publications in the open literature accounting for particle size, such as seen in the work of Agu et al. (Agu et al., 2019), or regarding the biomass effect over bubbles. In this respect, Fotovat et al. (Fotovat et al., 2015), were one of the first authors to detect bubbles using parallel fiber optics in the presence of biomass pellets.

This phenomenon is highly complex and has been studied using different combinations of particle sizes, particle types, added biomasses, fluid flow rates, feed compositions and reactor configurations (Fotovat et al., 2013; Grace and Harrison, 1967; Lim and Agarwal, 1992; Mori and Wen, 1975; Olowson and Almstedt, 1992; Valenzuela and Glicksman, 1985). However, to
progress in this research, one valuable approach is to study single bubbles in dense phase sand fluidized beds, tracking them throughout the bed. In addition, and as proposed in the present study, this single bubble dynamic analysis can also be developed using biomass pellets loaded in the bed of sand.

Given the need to account for the different fluidized bed dimensions, temperatures, and steam/air flows, the use of computational methods provides a valuable complement to experimental work (Fotovat et al., 2015). This is required to proceed with a cost-effectiveness scaling-up approach. Computational Fluid Dynamics (CFD) is a powerful tool and widely used computational method that allows the study of complex two-phase systems such as fluidized beds, among others.

Thus, there are three possible CFD strategies when simulating two-phase gas-particle systems (Ostermeier et al., 2019):

The Eulerian-Eulerian approach (Chen et al., 2013), known as the Two-Fluid Model (TFM), considers both the fluid and the solids as interpenetrating continuous phases. While this method has the advantage of not being computationally expensive, it is not able to account for solid-solid interactions and, as a result, misrepresents the dense phase.

The Eulerian-Lagrangian approach (Xu and Yu, 1997), designated as the Discrete Element or Discrete Particle Method (DEM or DPM), considers the fluid as a continuous phase while tracking every single particle and its interactions. DEM demands significant computational resources, while its use is limited to a restricted number of particles.

However, and as an alternative, one can consider a different Eulerian-Lagrangian approach, known as Multiphase Particle-in-Cell (MPPIC) Model. MPPIC uses computational particles
et al., 2015), treating the fluid as a continuum and the solids as a group of particles instead of individual particles. Identical physical properties are assigned to all particles in the groups, which are designated as computational particles.

While variations in these methodologies or combinations between these exist, these three basic categories remain as the building blocks of almost every strategy, used in the context of the computational fluid dynamics approach for multiphase gas-solid studies.

In the early 2000s, Snider (Snider, 2001; Snider et al., 2011) developed the MPPIC method that uses a fixed Eulerian grid. Lagrangian particles transport mass, momentum, and energy through this grid. Interactions between particles on the Eulerian grid are calculated with particle properties being interpolated in the selected mesh. (Pannala et al., 2010). CPFD Barracuda VR® (CPFD Software LLC, 2020) uses this CFD-MPPIC approach, providing faster calculations with an adequate level of accuracy (Liang et al., 2014). This software also allows the use of different drag models, as described later on page 6 in Section 2.2. Thus, by using this software, one can look more deeply into the possible value of these drag models available in the literature.

2.1 Single Bubble Rise Velocity-Size Correlations

Regarding bubble motion in fluidized beds, it has been argued that bubbles may be considered to behave as a bubbling liquid of low viscosity (Kunii and Levenspiel, 1991). This leads to the classic model of Davies and Taylor (Davies and Taylor, 1950), as expressed in Equation (1). According to this view, bubble rise velocity (BRV) depends only on two factors: the acceleration of gravity (g) and the bubble nose radius (Rn).
This model has been modified to adapt to the conditions of different experiments. In this regard, using experimental data from a 0.0152 m diameter bed with a particle size distribution between 150 µm and 400 µm, Davidson and Harrison (Davidson and Harrison, 1963) derived a model, Equation (2), valid for bubble diameter to bed diameter ratios inferior to 0.125 (0.055 m in the used reactor). Bubbles larger than this would be subjected to the vessel walls effect.

\[
BRV = 0.711 \sqrt{g d_{beq}} \tag{2}
\]

where \(d_{beq}\) is the diameter of an equivalent sphere with the same volume as the air volume contained in a bubble.

Later, Wallis (Wallis, 1969) formulated a variation of the Equation (2), by including the effect of the reactor walls for the 0.125 to 0.6 \(d_{beq}/D\) ratio as shown in Equation (3)

\[
BRV = \left(0.711 \sqrt{g d_{beq}}\right) 1.2 \exp \left(-1.49 \frac{d_{beq}}{D_{bed}}\right) \tag{3}
\]

where \(D_{bed}\) is the diameter of the sand column.

In a parallel effort, two models were developed by Rowe (Rowe and Partridge, 1965; Rowe and Yacono, 1976). The first one, Equation (4), applies for Geldart B type particles only, while the second one, Equation (5), includes particle diameter as a factor for Geldart type A and B particles.
\[ BRV = 1.02 \sqrt{gd_{beq}} \quad (4) \]

\[ BRV = (1.38 - 0.00182d_p) \sqrt{\frac{gd_{beq}}{2}} \quad (5) \]

As well, Allahwala and Potter reported an alternative model (Allahwala and Potter, 1979), Equation (6), which can be considered as well. This model uses as a secondary correction factor, the ratio of a bubble diameter over a reactor diameter with this being the argument of a hyperbolic tangent function.

\[ BRV = 0.35 \sqrt{gD_{bed}} \times \left( \tanh \left[ 3.6 \left( \frac{d_{beq}}{D_{bed}} \right)^{0.9} \right] \right)^{0.555} \quad (6) \]

Regarding model applicability, Karimipour and Pugsley (Karimipour and Pugsley, 2011) compared various sets of data to the available models described in Equations (1) to (6) and concluded that the best fitting was provided by Wallis’ model. One should notice that most of the models studied by Karimipour and Pugsley (Karimipour and Pugsley, 2011) were developed with type A and low size type B particles.
2.2 Computational Fluid Dynamic Modeling in Dense Sand Fluidized Beds Model

Equations

The development of CFD-MPPIC calculations in a dense phase sand fluidized bed requires the consideration of the following:

a) A continuity equation for the continuum gas phase (Snider, 2001) is expressed as:

$$\frac{\partial (\rho_f \theta_f)}{\partial t} + \nabla \cdot (\theta_f \rho_f \mathbf{u}_f) = 0$$

where $\rho_f$ represents the fluid’s density, $\theta_f$ is the fluid volume fraction, $t$ is the time and $\mathbf{u}_f$ is the fluid’s velocity.

A momentum conservation equation for the fluid (Snider, 2001) as expressed in Equation (8):

$$\frac{\partial (\theta_f \rho_f \mathbf{u}_f)}{\partial t} + \nabla \cdot (\theta_f \rho_f \mathbf{u}_f \mathbf{u}_f) = -\nabla p - \mathbf{F} + \theta_f \rho_f \mathbf{g} + \nabla (\theta_f \tau_f)$$

where $\rho_f$ is the fluid’s density, $p$ is the pressure, and $\mathbf{g}$ is the gravitational acceleration. $\mathbf{F}$ is the rate of momentum exchange per volume between the fluid and particle phases, calculated with Equation (9), and $\tau_f$ represents the fluid’s stress tensor as per Equation (10).

$$\mathbf{F} = -\iiint f \left[ m_p \left( \mathbf{D}_p (\mathbf{u}_f - \mathbf{u}_p) - \frac{\nabla p}{\rho_p} \right) + \mathbf{u}_p \frac{dm_p}{dt} \right] dm_p d\mathbf{u}_p dT_p$$

where $f$ represents the particle distribution function or PDF which is considered to be a function of the particle spatial location $\mathbf{x}_p$, particle velocity $\mathbf{u}_p$, particle mass $m_p$, particle temperature $T_p$, and time $t$. Thus, $f(\mathbf{x}_p, \mathbf{u}_p, m_p, T_p, t) d\mathbf{u}_p dm_p dT_p$ is the average number of particles per unit volume with velocities in the interval $(\mathbf{u}_p, \mathbf{u}_p + d\mathbf{u}_p)$, masses in the interval $(m_p, m_p + dm_p)$, and temperatures in the interval $(T_p, T_p + dT_p)$. $\mathbf{D}_p$ is the drag force function, $u_f$ represents the fluid’s velocity, $p$ is the pressure, and $\rho_p$ is the particle’s density.
A constitutive equation for the non-hydrostatic component of the stress, \( \tau_f \), for the “ij” indexes as:

\[
\tau_{f,ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \delta_{ij} \frac{\partial u_k}{\partial x_k}
\]

(10)

with \( \mu \) as the shear viscosity, \( x_i \) and \( x_j \) represent the spatial locations of the \( i \) and \( j \) respectively, and \( u_i \) and \( u_j \) represent the velocity of the \( i \) and \( j \) elements, respectively.

Assumptions included in these equations for the fluid phase are as follows:

a) A laminar and isothermal flow,

b) A momentum equation that does not take into account the viscous molecular diffusion in the fluid, retaining, however, the viscous drag between fluid and particles using a drag force model.

On the other hand, the particle phase is described using a particle probability distribution function designated as \( \phi(x, u_p, \rho_p, \Omega_p, t) \), where \( x \) provides the particle position, \( u_p \) the particle velocity, \( \rho_p \) the particle density, and \( \Omega_p \) the particle volume. It is assumed that the mass of each particle remains constant over time and that there is no mass transport between particles and the fluid phase.

Furthermore, the time evolution of the distribution function \( \phi \) is obtained by solving the Liouville Equation (11):

\[
\frac{\partial \phi}{\partial t} + \nabla \cdot (\phi u_p) + \nabla u_p \cdot (\phi A) = 0
\]

(11)

with \( \nabla u_p \) being the divergence operator with respect to velocity, and \( A \) is the discrete particle acceleration term that can be defined as follows:
\[ A = D_p(u_f - u_p) - \frac{1}{\rho_p} \nabla \rho + g - \frac{1}{\theta_p \rho_p} \nabla \tau + \frac{\overline{u_f} - \overline{u_p}}{\tau_D} \]  \hspace{1cm} (12)

Regarding Equation (12), the first term in the right side accounts for the aerodynamic drag, the second for the pressure gradient, the third for the gravitational force, and the last one for the interparticle stress.

Furthermore, the drag force imposed on the particle by the fluid depends on the interphase drag coefficient, defined as follows:

\[ D_p = \frac{3}{8} C_d \rho_f |u_f - u_p| \rho_p^\beta \]  \hspace{1cm} (13)

with \( C_d \) being a drag coefficient calculated accordingly with the selected drag models.

### 2.3 Particle-to-Particle Interactions

Regarding particle-to-particle interactions, Equation (14) establishes the most efficient computational particle stress function as follows:

\[ \tau(\theta_p) = \frac{10 P_s \theta_p^\beta}{\max[\theta_{CP} - \theta_p, \epsilon(1 - \theta_p) \theta_p]} \]  \hspace{1cm} (14)

with \( P_s \) being a parameter with units of pressure, \( \theta_{CP} \) a close-packed particle volume fraction, \( \beta \) a parameter with a 2 to 5 recommended value (Auzerais et al., 1988), and \( \epsilon \) a \( 10^{-7} \) parameter included eliminating the singularity in the close-packed configuration (Harris and Crighton, 1994). Equation (14) is based on the work of Harris and Crighton (Harris and Crighton, 1994), and depends on particle concentration, disregarding particle size, and velocity effects. While more complex models have been developed (Ding and Gidaspow, 1990; Jenkins and Savage, 1983; Lun et al., 1984), they involve a greater computational time cost. Due to this, the most efficient computational particle stress function proposed by Snider (Snider, 2001; Snider et al., 2011) was used in the calculations developed.
2.4 Drag Models

The CPFD Barracuda VR® software uses drag force calculations for simulations, utilizing as a reference, the Stokes Drag Coefficient. Due to this, all studied models are multiplied by the $24/\text{Re}$ factor. These drag models are available in CPFD Barracuda VR® and are listed in the next Sections.

2.4.1 Wen-Yu Drag Model

The Wen-Yu Model (Kunii and Levenspiel, 1991), reported in Equation (15) is used frequently in diluted phase beds:

$$C_d = \begin{cases} 
\frac{24}{\text{Re}} \theta_f^{2.65} & \text{Re} < 0.5 \\
\frac{24}{\text{Re}} \theta_f^{2.65} (1 + 0.15 \text{Re}^{0.687}) & 0.5 \leq \text{Re} \leq 1000 \\
0.44 \theta_f^{2.65} & \text{Re} > 1000 
\end{cases}$$

Equation (15)

where $\theta_f$ is the fluid volume fraction, and $\text{Re}$ is the Reynolds Number.

2.4.2 Ergun Drag Model

The Ergun Model (Kunii and Levenspiel, 1991), described by Equation (16) is mostly used for dense phase beds:

$$D_p = 0.5 \left( \frac{180 \theta_p}{\theta_f \text{Re}} + 2 \right) \frac{\rho_f |u_f - u_p|}{\rho_p r_p}$$

Equation (16)

2.4.3 Wen-Yu/Ergun Blend Drag Model

The Wen-Yu/Ergun Model (Dey et al., 2015), involves a combination of drag models described in Sections 2.4.1 and 2.4.2. Given the Wen-Yu Model works better with smaller particle fractions and the Ergun Drag Model is more appropriated for greater particle fractions, the
following approximation was proposed for the evaluation of the drag force applied by the fluid over the particle:

\[
D_p = \begin{cases} 
  D_{p1} & \theta_p < 0.75\theta_{CP} \\
  (D_{p2} - D_{p1}) \left( \frac{\theta_p - 0.75\theta_{CP}}{0.85\theta_{CP} - 0.75\theta_{CP}} \right) & 0.75\theta_{CP} \geq \theta_p \geq 0.85\theta_{CP} \\
  D_{p2} & \theta_p > 0.85\theta_{CP} 
\end{cases}
\]  

(17)

where \(\theta_p\) represents the particle volume fraction, \(\theta_{CP}\) is the close-packed particle volume fraction, \(D_{p1}\) is the Wen-Yu Drag Function given by combining Equations (13) and (15) and \(D_{p2}\) is the Ergun Drag Function given by Equation (16).

2.4.4 Turton and Levenspiel’s Drag Model

The Turton and Levenspiel’s Drag Model (Levenspiel and Haider, 1989) considers a specific model applicable to the fluidization of fine particles (~100 μm). This model is frequently used to calculate drag coefficients for Geldart Type A particles.

\[
C_d = \frac{24}{Re} \left[ 1 + 0.173Re^{0.657} \right] + \frac{0.413}{1 + 16300Re^{-1.09}} \theta_f^{2.65} 
\]

(18)

2.4.5 Syamlal O’Brien Drag Model

The drag model described with Equations (19) to (21) (Syamlal and O’Brien, 1988), was derived from the Richardson-Zaki type velocity-voyage correlation, based on two parameters. These are the Reynolds number and the void fraction. This model is appropriate for only Geldart Group B particles (ANSYS, 2015).

\[
C_d = \frac{24}{Re} \left[ \frac{1}{V_{rp}^2} \left( 0.63 + \frac{V_{rp}}{Re} \right)^2 \right] 
\]

(19)
where

\[
V_{rp} = 0.5 \left( \theta_f^{1.14} - 0.06Re + \sqrt{(0.06Re)^2 + 0.12Re(2B - \theta_f^{1.14}) + (\theta_f^{4.14})^2} \right)
\]  
(20)

\[
B = \begin{cases} 
0.8\theta_f^{1.28} & \theta_f \leq 0.85 \\
\theta_f^{2.65} & \theta_f > 0.85 
\end{cases}
\]  
(21)

2.4.6 Non-Spherical Ganser Drag Model

The Non-Spherical Ganser Drag Model (Ganser, 1993) was specifically developed for the accounting of the irregular particle shape. It was assumed that every isolated particle experiences Stokes’ and Newton’s regimes. The Stokes regime involves a drag coefficient inversely proportional to fluid velocity, while the Newton yields a drag proportional to the square of the fluid velocity. This model can be expressed as follows:

\[
C_d = \theta_f^{-2.65} K_2 \left[ \frac{24}{ReK_1 K_2} (1 + c_0 (ReK_1 K_2)^{0.6567}) + \frac{0.43056}{1 + \frac{3305}{ReK_1 K_2}} \right]
\]
(22)

with

\[
K_1 = \frac{3}{1 + 2\psi^{-0.5}}, \quad K_2 = 10^{1.8148(- \log \psi)^{0.5743}}
\]
(23)

where \(\psi\) represents the particle sphericity.

2.4.7 Parameterized Syamlal-O’Brien Drag Model

The Syamlal-O’Brien Model (Syamlal and O’Brien, 1988) provides a drag coefficient adjusted to an experimentally determined minimum fluidization velocity \(u_{mf}\) as follows:

\[
C_D = \left( \frac{0.63}{V_{rp}} + \frac{4.8}{\sqrt{V_{rp} Re_{single}}} \right)^2
\]
(24)
with $V_{rp}$ given by Equation (20) and $Re_{single}$ being the Reynolds Number for a single particle at terminal settling conditions,

$$Re_{single} = \left[ \frac{\left( 4.8^2 + 2.52 \sqrt{\frac{4Ar}{3}} \right)^{0.5}}{1.26} - 4.8 \right]^2$$  \hspace{1cm} (25)

On the other hand, the Archimedes number ($Ar$) can be considered to be a function of both the drag coefficient and of the $Re_{single}$

$$Ar = \frac{3}{4} C_D Re_{single}^2$$  \hspace{1cm} (26)

Furthermore, this $Re_{single}$ can be related to the $Re_{min}$ at minimum fluidization as:

$$Re_{min} = Re_{single} \left[ A + 0.06 B Re_{single} \right]$$  \hspace{1cm} (27)

with the constant $A = \theta_f^{4.14}$.

On this basis, Syamlal O’Brien Model proposes to adjust $c_1$ and $d_1$ parameters using (Syamlal and O’Brien, 1987).

$$B = \begin{cases} 
c_1 \theta_f^{1.28} & \text{if } \theta_f \leq 0.85 \\
\theta_f^{d_1} & \text{if } \theta_f > 0.85 
\end{cases}$$  \hspace{1cm} (28)

With:

$$d_1 = 1.28 + \frac{\log_{10} c_1}{\log_{10} 0.85}$$  \hspace{1cm} (29)

### 2.4.8 EMMS-Yang-2004 Drag Model

The EMMS-Yang-2004 model used in this study (Yang et al., 2004), has its constants generated for the following conditions based on the Li and Kwauk (Li and Kwauk, 1994) experiments developed as follows: a) air at atmospheric conditions, b) 54 µm mono-sized particles,
c) particle density of 930 kg/m3, d) fluid superficial velocity of 1.52 m/s, e) Solids Flux of 14.3 kg/m²s

The Drag force for this Model is calculated using Equation (30):

\[
D = \frac{9}{2} \frac{\mu_f}{\rho_p r_p^2} f_e
\]  

(30)

where \( f_e \) is given by Equation (31) with three possible options for fluid volume fraction.

\[
f_e = \begin{cases} 
\frac{1}{18\theta_f} \left( \frac{150}{\theta_f} \frac{\theta_p}{\theta_f} + 1.75Re \right) & \theta_f < 0.74 \\
(1 + 0.15Re^{0.687})\omega & \theta_f \geq 0.74 \text{ and } Re < 1000 \\
\frac{Re}{24} \omega & \theta_f \geq 0.74 \text{ and } \geq 1000
\end{cases}
\]

(31)

where \( \theta_f \) represents the fluid volume fraction, \( \theta_p \) the particle volume fraction, \( Re \) the Reynolds Number and \( \omega \) is defined by Equation (32) as,

\[
\omega = \begin{cases} 
-0.576 + \frac{0.0214}{4(\theta_f + 0.7463)^2 + 0.0044} & 0.74 \leq \theta_f < 0.82 \\
-0.0101 + \frac{0.0038}{4(\theta_f + 0.7789)^2 + 0.0040} & 0.82 \leq \theta_f \leq 0.97 \\
-31.8295 + 32.8295\theta_f & 0.97 \leq \theta_f \leq 1
\end{cases}
\]

(32)

Given the various decision-making steps for calculating \( f_e \) and \( \omega \), this model is computationally consuming when compared to the other model alternatives reviewed earlier in this section.
2.5 Conclusions.

Thus, and despite the reported progress, there is a lack of comprehensive bubble models in dense phase fluidized beds using Geldart type B powders, with and without added biomass. Given this shortcoming, studies such as in the present study are required, where optical probe data and video micro-camera images are concurrently considered. This approach can lead to establishing a fundamentally based understanding of bubble dynamics in fluidized beds with different biomass loadings.

In this regard, given the advantages of limited computational cost and accuracy, the CFD-MPPIC method was selected in this research for studying single bubbles in a dense phase sand fluidized bed gasifier with loaded biomass pellets and compare experimental and numerical results. We are not aware of a similar contribution in the open literature.
Chapter 3: **Scope of the Research**

The overall objective of the present Ph.D. dissertation is to expand our knowledge on the fluid dynamics of sand fluidized bed gasifiers by analyzing the behavior of bubbles. To address this, we are particularly interested in tracking bubbles generated in a bed of irregular sand particles, and in assessing the effect of biomass addition. It is proposed to accomplish this by using both experimental and numerical methods in order to study a) bubble size, b) bubble velocity, and c) bubble shape.

The anticipated originality of this study resides in the tracking of bubbles in a sand fluidized bed, using both CREC Optiprobies and a video camera. This is done to establish the effect of biomass pellets in a sand fluidized gasifier unit.

Furthermore, the expected outcomes of this research are as follows: a) An experimental study of how single bubble dynamics are affected by biomass, b) A theoretical study via a numerical CFD-MPPIC analysis of the same bubble phenomenon, c) A systematic comparison of experimental and theoretical data, with the aim of validating a CFD-MPPIC based model.

### 3.1 Particular Objectives

Based on the overall objectives, the following particular objectives are set for this study:

a) To establish a geometrical model of the bubble that resembles closely to the actual shape observed with non-intrusive technologies like X-Ray and CT scans.

b) To develop an experimental methodology to inject single bubbles and measure them with the combined CREC-Optiprobies and video camera, in a Cold Model Unit of a sand fluidized bed gasifier of 0.44 m diameter. This unit is filled with sand with a Sauter Mean Diameter (MSD) of 520 µm.
c) To set a data treatment method to process the data from the experimental system, automatically while setting baselines for each voltage peak, generated by a single bubble while crossing the CREC-Optiprobe control volume.

d) To measure single bubbles in the absence of biomass using air mass balances and to do this for every single bubble studied.

e) To measure and analyze single bubble parameters in the presence of biomass pellets having a 2.7 cm length and a 0.7 cm diameter.

f) To compare the measured bubbles, with and without biomass with reported correlations, predicting bubble rise velocity as a function of bubble size. To propose, if needed, modified correlations to better represent the influence of biomass pellets addition.

g) To find with the help of a CFD-MPPIC simulation, drag models, and other input parameters required to reproduce the experimentally measured single bubbles.

h) To develop a novel methodology to treat CFD-MPPIC data, extracting information from the images produced from the simulation.

i) To replicate with the validated CFD-MPPIC simulation, the experimentally obtained single bubble parameters, with and without the addition of biomass.
3.2 Accomplishments of Research.

This research project has yielded so far one published paper, one graphical abstract published on a journal cover, and one manuscript submitted for publication, all of them in reputable chemical engineering journals. There is also one refereed abstract, which has been presented and published in the proceedings of an internationally prestigious conference and another to be published in the near future. There is also the expectation of completing and submitting a third paper for a refereed international following the Ph.D. thesis defense.

a) Manuscript 1 entitled “Single-Bubble Dynamics in a Dense Phase Sand Fluidized Bed Biomass Gasification Environment.” This article was published in *Industrial and Engineering Chemistry Research*, volume 59, issue 13, pages 5601-5614 Publisher: American Chemical Society, March 2020. It reports the results of the single bubble experimental work of this study. Chapters 4, 5, and 7 of this dissertation are based on this manuscript.

b) Manuscript 2 entitled “Single Bubble in a 3D Sand Fluidized Bed Gasifier Environment: A CFD-MPPIC Simulation”. This manuscript was submitted for publication in April 2020 to *Chemical Engineering Science*. Publisher: Elsevier, Chapters 6, and 8 report the advances presented in this manuscript.

d) **Refereed Abstract 1.** A refereed abstract extracted from the first manuscript was published in **2019 AIChe Annual Meeting Proceedings. ISBN: 978-0-8169-1112-7**

e) **Refereed Abstract 2.** This work has been accepted as a lecture in the **11th International Symposium on Catalysis in Multiphase Reactors (CAMURE11),** and its abstract will be published in its proceedings.

f) **Manuscript 3** entitled “Bubbling Sand Fluidized Bed for Biomass Gasification: CFD-MPPIC Simulation and Experimental Studies.” This manuscript will be submitted in July 2020 to a reputable refereed international journal. Chapters 10 reports the main results to be included.
Chapter 4: **Experimental Methods**

The experimental setup used in the present study involved a sand fluidized bed unit operated at room temperature, designated as a Gasifier Cold Model Unit. Its construction, as detailed in the upcoming sections, allowed us to study the hydrodynamics of the dense and dilute phases during fluidization of sand with and without biomass being present. Multiple sensors allowed one to measure the pressure and localized particle volume fractions, while video images captured the state of the bed surface.

This chapter describes the details of the experimental system configuration, the sand properties, the biomass, the sensors, and the single bubble injection system.

4.1 **The Fluidized Bed Gasifier Simulator.**

The cold model of the fluidized bed gasifier (Figure 4-1) consisted of a column divided into 3 sections. The lowest section was designated as the wind box. A 20 cm height plexiglass cylinder with a 44 cm diameter constituted the wind box. On top of it, there was a perforated plate, which served as an air distributor.

The distributor plate was manufactured out of steel with 37 small short tubes. Each tube had a 2.5 cm height, a 1.1 cm radius, and eight (8) circumferentially and equally distributed 2 mm diameter holes pointing toward its center. Additional information can be found in Section 4.2 of the present Ph.D. dissertation. This distributor served two functions: a) It kept the sand in the main sections from falling into the wind box, and b) It provided an evenly distributed airflow fed from the wind box into the main unit bed section.
This main unit bed section contained both the sand and the biomass. It had 4 ports that allowed the insertion of the CREC-Optiprobes to measure the local void fractions and bubble velocities. It was made of plexiglass, with a 44 cm diameter and a 120 cm height.

The unit was equipped as well, with an upper metallic section having a 70.6 cm inner diameter. It had a side sand loading port and at the top, a camera insertion port. The unit gas exit was connected to a cyclone. This cyclone collected sand particles that escaped from the freeboard, returning them directly to the fluidized bed via an external dipleg. One should also note that the cyclone gas exit was connected to the building exhaust system. This building exhaust system included a particle filter that removed small particles.

![Figure 4-1. Schematics of the Fluidized Bed Gasifier Simulator Describing Unit Dimensions, Positioning of the Video Camera, Location of the CREC Optiprobes, and the Bubble Injection System.](image-url)
The airflow was measured at the entrance to the Wind Box of the Gasifier Cold Model Unit using a rotameter graduated from 0 to 180 SCFM in steps of 2 SCFM. The unit described in Figure 4-1 was also equipped with one Omega PX409-015G5V (0-15PSI) and three Omega PX409-2.5G5V (0-5PSI) pressure sensors which allowed one to measure the pressure in the following locations: a) the unit wind box, b) the middle of the bed above the bubble injection point, c) above and close to the bed surface and d) 40 cm above the bed surface.

4.2 Graphical Representation of the Distributor

The distributor used in the present study was briefly described in Section 4.1, with Figure 4-2, providing an additional description of its characteristics.

![Fluidized Bed Distributor Plate](image)

*Figure 4-2. Fluidized Bed Distributor Plate Used in the Present Study: a) The steel plate has 37 short tubes cylinders with a 2.5 cm height and a 1.1 cm radius. b) Each tube is equipped with 8 circumferentially and equally distributed 2 mm nozzles pointing toward its center.*

4.3 Sand Particles

The bed was composed of silica sand (SiO$_2$) with a particle size distribution (PSD) between 240 µm to 955 µm and having a 586 µm size on average, as shown in Figure 4-3. According to Geldard’s classification, the sand used was comprised of group B and group D type of particles.
It is reported by Geldard, that the minimum bubbling velocity of groups B and D particles is lower than the minimum fluidization velocity. Therefore, one cannot fluidize these types of sand particles without forming bubbles.

Figure 4-3. Sand Particle Size Distribution.

4.4 Biomass Particles

Biomass pellets as the ones used in the ICAFE Costa Rica gasifier are the result of compressing coffee waste broza particles. Figure 4-4 shows an example of these pellets having a length of 2 to 4 cm and a diameter of 0.8 cm (Erlich and Fransson, 2011; Torres et al., 2019). However, in the present study and to emulate these broza pellets, truncated pinewood cylinder pellets (Figure 4-5) having a length of 2.7 cm and a diameter of 0.79 cm were fabricated and used. They had an apparent density deviating less than 5% from the ones employed in a Costa Rica gasifier.
These wood pellets were introduced into the bed from the top-loading port and rested initially on the surface of the sand bed. Later, the bed was fluidized for 5 to 10 minutes using a superficial air velocity of 0.28 m/s. This was done to mix the biomass pellets into the bed and achieve homogeneity before the experiments were performed. Visual observations allowed one to confirm that this condition was achieved.

4.5 The CREC-Optiprobes

The detection of the bubbles in the present study involved the use of the CREC-Optiprobe system. In this setup, the laser was transported via a fiber optic cable to a GRIN (Graded Refraction Index) lens located at the tip of the CREC-Optiprobe. The GRIN lens focused the beam to a focal point placed 5 mm away in front of the Optiprobe tip. Thus, when the laser beam hit a sand particle, the light was reflected towards the receiver fiber optic cable, placed adjacent to the GRIN lens, as
is shown in Figure 4-6. This return cable was connected to a sensor that received the light from the reflection. A voltage was generated, and the resulting signal was converted in an A/D signal converter and later recorded. Additional details of this CREC-Optiprobe system can be found in the works of Nova, and Lanza (Lanza, 2015; Lanza et al., 2012; Nova et al., 2004).

Figure 4-6(a) and Figure 4-6(b) describe the CREC-Optiprobe operation as an on-off detector with the following taking place: a) When the emulsion phase filled the control volume the transmitted laser rays reached the receiver fiber (“On” condition), b) When a bubble was present in the measuring volume, the laser rays were not reflected (“Off” condition).

Figure 4-6. a) CREC-Optiprobe under “On” Operating Condition, b) CREC-Optiprobe under “Off” Operating Condition. The measurement condition represented is close to the unit wall. The same principle was applied at other radial positions.
Thus, when two sets of vertically aligned CREC-Optiprobes with a selected 5.4 mm separation were used as shown in Figure 4-7, the time-delay between “off” CREC-Optiprobes signals allowed calculating the bubble rise velocity (BRV) as reported in Equation (33). It was hypothesized that signal interference between probes could be neglected. This was given the wide angles, and much larger optical paths required for focal region reflected rays from CREC Optiprobe 1 to reach the Receiver Fiber of CREC Optiprobe 2, and vice versa.

Additionally, and once the BRV was calculated, the elapsed time between the beginning and the end of the “off” signal (width of the “off” signal) was divided by the BRV. This quotient was defined as the bubble axial chord (BAC), as shown in Equation (34).

\[
BRV = \frac{\text{intersensor distance}}{\text{time delay}} \tag{33}
\]

\[
BAC = \frac{\text{width of the "off" signal}}{BRV} \tag{34}
\]

*Figure 4-7. Assembly of CREC-Optiprobe System.*
Furthermore, the CREC-Optiprobe allowed calculating the cumulative time when the measuring volume was filled with a dense phase as per Equation (35). This was done by subtracting from the total sampling time the sum of the individual duration of individual bubble contacts with the CREC Optiprobe.

\[
(1 - e) = \frac{t_{\text{total}} - \sum \Delta t_{\text{bubble}}}{t_{\text{total}}}
\]  

Thus, the CREC-Optiprobe system of the present study allowed one to simultaneously calculate the bubble rise velocity, the bubble axial chord, and the void fraction.

### 4.6 Single Bubble Detection System

*Figure 4-8. Details of the Single Bubble Injection System Developed for this Study. The positions of the Camera and its Field of View, the CREC Optiprobe System, the Injection System are Illustrated.*
Figure 4-8 describes the fluidized bed with the instrumentation used in the present research. At the bottom section of this unit, at 12 cm above the distributor plate, there was a steel tube with a 3 mm nozzle. The tip of this small nozzle was placed at the center of the cylindrical unit. This tube was connected to a 150 cm³ stainless steel bottle and a pressurized air cylinder. The manometer of the air cylinder allowed the control of the amount of air introduced into the stainless-steel bottle, and as a result, the air volume injected as bubbles into the fluidized bed reactor. One should also note that while air is injected, pressurized air is being fed through the distributor plate at a minimum fluidization velocity (0.17 m/s). This avoids interference with any other bubbles formed inside the bed. Experiments were developed under conditions free of pellet segregation as attested by the visual observation of the bed surface and unchanged bubble sizes or velocities as recorded by the CREC Optiprobes during the 5 min of the run.

Furthermore, and as also shown in Figure 4-8, at the top of the reactor, a video camera hung vertically 0.80 m above the bed surface. This camera recorded images of bubbles reaching the bed surface, as well as bubble breakage, providing frontal bubble dimensions.

Every time a bubble was injected from the gas injector bottle into the bed at minimum fluidization conditions, the CREC-Optiprobe system measured its axial chord (BAC). As well, the video camera-generated video frames of the frontal diameter of the injected bubble. In addition, and to make sure that the BAC and bubble front diameter measured corresponded to each other, measurements with the CREC Optiprobes were performed at about 1 cm above the bed surface.

One should notice that the stainless-steel bottle could be loaded with different amounts of air depending on its pressure, forming as a result, bubbles of different volumes. In the present study, 138 kPa, 207 kPa, 276 kPa, 345 kPa, and 414 kPa (gauge pressures) were employed in order to investigate bubble sizes in the 0.04-0.07 m range.
4.7 Conclusions

a) A sand fluidized bed system with its auxiliary measurement equipment was effectively implemented to study bubble dynamics.

b) The successfully engineered unit allowed reliable bubble injections with formed bubbles in the 4 cm to 10 cm diameter range.

c) The implemented measurement system, with CREC Optiprobes and video camera, allowed the satisfactory evaluation of both the BAC (Bubble Axial Chord) and bubble frontal radii.

d) The successful tracking of these two essential bubble geometrical parameters provided essential data for sand fluidized bed model validation.
Chapter 5: Development of the Experimental Hybrid Spherical Cap Model

Given the experimental system capabilities for the present study at the CREC-UWO, as detailed in the previous chapter, it was possible to track single bubbles in a sand fluidized bed. Furthermore, and to be able to determine the bubble velocity and bubble size, a geometrical model had to be established to calculate bubble volume.

In this respect, if one assumes that single bubbles are perfect spheres, the bubble radius suffices to calculate the bubble volume. However, and because single bubbles are not spherical, other additional considerations are required.

Thus, the development of a geometrical bubble model was needed to correlate in situ measurements of the experimentally obtained bubble with the single bubble volume from the simulation. This proposed model is a combination of assumptions and experimental observations taken from the bibliography. This chapter explains step-by-step the derivation of such a model and its application to calculate the Bubble Axial Chord (BAC) and the bubble radius (R) for a given volume. The same calculation can be performed in reverse when data such as the-BAC and R are available experimentally for the calculation of the bubble volume.

5.1 Geometrical Considerations

The study of sand fluidized bed fluid dynamics in biomass gasifiers requires bubble size, bubble velocity, and bubble shape determination. Given the focus of the first part of this Ph.D. Dissertation on single bubbles analysis, a geometrical model was developed to theoretically determine a standardized size and shape of the bubble and to compare it against experimental measurements. With this accomplished, and using the experimentally obtained data, a bubble
volume was calculated and compared to the experimentally injected air volume. This was done to validate the proposed model via the mass balance closure.

The proposed model is based on the following assumptions:

a) The HESC model is a perfect sphere with two separate sections.

b) These two sections are the air pocket (or bubble) and the wake (a region with dragged solid particles).

c) The separation between these two sections is a well-defined discrete zone called the bubble wake interface.

The intent of this bubble model is to provide a phenomenologically based framework for the analysis of bubble flow in fully fluidized sand beds with multiple coexisting bubbles.

In this respect, one can consider $V_T$, which represents the total spherical volume for a $V_b$, which stands for the portion of the sphere filled with air (bubble volume) and a $V_w$, which denotes the wake volume filled with solid particles. Thus, by using bubble volume conservation and geometrical considerations, Equations (36) and (38) describe the bubble mathematically as follows:

\[ V_T = V_b + V_w = V_b(1 + f_w) \]  
\[ f_w = \frac{V_w}{V_b} \]  
\[ R = \sqrt[3]{\frac{3V_T}{4\pi}} = \sqrt[3]{\frac{3V_b(1 + f_w)}{4\pi}} \]

with $f_w$ representing the bubble wake fraction, and $R$ denoting the bubble cap frontal radius.
This modeling approach is consistent with previous studies (Grace and Harrison, 1967; Puncochar et al., 2019). It is assumed that the front section of bubbles can be considered as spherical caps, with the back fraction of these bubbles being represented as wakes, as shown in Figure 5-1.

![Figure 5-1. Bubble Cap Model with the Flat Bubble-Wake Interface. The Height of the Air Pocket is Called the Bubble Axial Chord (BAC), and the Sphere Radius is Designated as R.](image)

In addition, and based on geometrical considerations, one can also state that the volume of the bubble cap is related to the bubble radius and its height as follows:

\[
V_b = \frac{\pi (BAC)^2}{3} (3R - BAC)
\]  

Thus, by knowing the bubble radius from Equation (38) and using Equation (39), one can obtain the BAC (Bubble Axial Chord) values via a non-linear regression calculation. However, and as reported by (Boyce et al., 2019), the proposed bubble model requires enhancements, as shown in Figure 5-2, with the back of the bubble being represented with an anticipated uneven (non-flat) bubble-wake interface.
Figure 5-2. 2D Model Representation of the Expected Bubble Wake Interface in Accordance with the Observed Images.

Figure 5-3. Images of a Single Bubble Taken from Boyce et al. The Bubble-Wake has an Uneven (non-flat) Interface.
This representation of the bubble wake interface is consistent with the studies of several authors, as shown in Figure 5-3 (Boyce et al., 2019; Grace and Harrison, 1967; Kunii and Levenspiel, 1991). Thus, to generate this irregular interface 2D bubble cap shape, the following two equations are considered: a) Equation (40) for the outer circular shape of the bubble and b) Equation (41) for the double-parabola that shapes the irregular bubble wake interface.

Outer Spherical Shape
\[ x^2 + y^2 = R^2 \] (40)

Inner Bubble Wake Interface Based on a Double-Parabola Representation
\[ y = c_1 x^4 + c_2 x^2 + c_3 \] (41)
with \( x \) and \( y \) being the axes of the 2D projection image of the sphere in Cartesian coordinates.

Once these equations are chosen to provide the 2D projection, this projection can be rotated to generate a solid sphere (bubble and wake) using the Shell Method of Solids of Revolution (Courant, 1936). From the use of this method, Equations (42) and (43) are derived as follows:

\[ V_b = \int_0^R 2\pi x \left( \sqrt{R^2 - x^2} - (c_1 x^4 + c_2 x^2 + c_3) \right) dx \] (42)

\[ V_w = \int_0^R 2\pi x \left( \sqrt{R^2 - x^2} + (c_1 x^4 + c_2 x^2 + c_3) \right) dx \] (43)

By integrating Equations (42) and (43) analytically, we obtain (44) and (45):

\[ V_b = \frac{1}{6} \pi (-2c_1 R^6 - 3c_2 R^4 - 6c_3 R^2 + 4R^3) \] (44)

\[ V_w = \frac{1}{6} \pi (2c_1 R^6 + 3c_2 R^4 + 6c_3 R^2 + 4R^3) \] (45)

By inserting (44) and (45) into Equation (37), the following results are obtained:
\[-2R^6(f_w + 1)c_1 - 3R^4(f_w + 1)c_2 - 6R^2(f_w + 1)c_3 + 4R^3(f_w - 1) = 0 \quad (46)\]

Furthermore, by considering that the radius of the bubble is the root of Equation (40), this gives the following Equation (47):

\[c_1 R^4 + c_2 R^2 + c_3 = 0 \quad (47)\]

By multiplying Equation (47) by \(2R^4(f_w + 1)\) and adding it to Equation (46), this yields:

\[c_1 = \frac{-R^2c_2 - c_3}{R^4} \quad (48)\]

\[c_2 = \frac{4R^2(f_w + 1)c_3 - 4R^3(f_w - 1)}{-R^4(f_w + 1)} \quad (49)\]

This algebraic process leads to a set of two equations. These are Equations (48) and (49) with three parameters \((c_1, c_2, \text{ and } c_3)\). Thus, once \(c_3\) is set, \(c_1\) and \(c_2\) can be calculated. Then, using Matlab, the value of the \(c_3\) parameter can be adjusted until the \(\alpha\) angle between the bubble center and the two minimums of the inner bubble interface function, Equation (41), as shown in Figure 5-2 is 90°. This 90° angle is equivalent to a 122° wake angle \((\theta_w)\) consistent with the results obtained by Rowe and Partridge (Rowe and Partridge, 1965). These authors found this angle to be 124° for sand particles of close size, with a standard deviation of 8°.

Once the value for \(c_3\) complies with the wake angle condition, a theoretical BAC value can be calculated using Equation (50):

\[BAC = c_3 + R \quad (50)\]

On this basis, and in agreement with (Rowe and Partridge, 1965), the wake fraction \(f_w\) could be assessed to be 0.26.
Furthermore, and regarding the significance of these findings for the present study, one can see that once the volume of the injected bubble is established, $c_1$, $c_2$, and $c_3$, the R radius of the sphere and the BAC can be calculated.

This process of calculation gives a theoretically derived BAC and bubble radius, which can be compared with experimentally observed values. On this basis, the model of the present study can be analyzed and validated.

5.2 Conclusions

a) A geometrical model for the spherical bubble wake system was successfully developed.

b) The novel HESC model includes an interface between the bubble and the bubble wake, with this interface being consistent with those observed with non-intrusive analysis methods.

c) The HESC model allows the prediction of the BAC and the R of a bubble, given that the amount of air injected is known.

d) The HESC model allows the volume calculation of a single bubble by knowing only two experimental measured parameters: Bubble Radius (R) and Bubble Axial Chord (BAC).

e) This HESC model can be validated by showing that the calculated air volume agrees with injected air volume.
Chapter 6: **Experimental Data Analysis**

The raw data output from the CREC Optiprobe system and the video images recorded must be processed in order to calculate the following: bubble size, bubble shape, and bubble velocity data. Additionally, the noise in the voltage signal at the exit of the CREC Optiprobes must be removed. Signal noise from the CREC Optiprobes can be created by probe vibrations and secondary reflections, as well as by light scattering in the measuring control volume. Therefore, a process must be implemented to clean the voltage signals, to find peaks generated by bubbles crossing the control volume, and to set an appropriate baseline for each one of them. On the other hand, the number of pixels indicating the size of the bubble, as recorded by the video camera, must be related to a frontal bubble measurement.

This chapter provides details of the experimental data treatment, the baseline setting, the noise reduction, and the video recording photo frames measuring. This treatment and calculations are applied to the raw experimental data.

### 6.1 Baseline Determination for the Bubble Axial Chord Measurement

The CREC-Optiprobe system generates a continuous voltage signal that varies from 0 to 5 V. The recorded frequency for these experiments was 1000HZ. One should note that the obtained data shows a train of signals averaging around 1.5 V with sudden drops reaching almost zero. These drops are the so-called “inverted” peaks, related to bubbles. This raw signal is noisy, with this being due to several factors. This creates a need for removing noise. To do so, a baseline setting method must be proposed. This allows one to obtain a new signal with signal noise influence being minimized.
Figure 6-1 describes typical peaks recorded using the CREC-Optiprobes. As one can see, the peak signal shapes recorded were close to trapezoids, with the narrow side of these trapezoids being on the signal bottom and the wide side being on the signal top. This shows both front and wake bubble effects.

![Figure 6-1. Typical Observed Voltage Changes as Recorded by the CREC-Optiprobes (Probes 1 and 2) in the Sand Fluidized Bed. Signals reported show the characteristics shaped trapezoidal peaks, which occur when bubbles come into contact with the CREC-Optiprobes.](image)

Given the above, setting the signal baseline offers challenges. A possible approach to setting the baseline is to make signal height adjustments until the injected gas volume matches the calculated bubble volume. This method considers both bubble chord and bubble frontal radius measured parameters. To accomplish this, a calculation using MATLAB was developed. It was used to obtain the time series signals and involved the following:
a) The first step (refer to Figure 6-2): The original signal is transformed into a “new” signal, with all signal values surpassing the signal average being deleted.

b) The second step (refer to Figure 6-3): The “new” signal is normalized using the raw signal average as its maximum. Thus, following normalization, all peak intensities, considered for further analysis vary in 0 to 1 range.

c) The third step: All shallow peaks with a normalized signal value smaller than 0.5 are removed for further analysis.

Following this procedure, the time shift for each bubble peak was defined by cross-correlating signals from the lower and upper CREC-Optiprobes, by using a cross-correlation function. After this step, the width of each peak was calculated, using the anticipated undisturbed signal of the lower probe. The time delay, given the known distance between sensors in the CREC-Optiprobe system, allowed one to calculate Bubble Rise Velocity (BRV) as per Equation (33), and the Bubble Axial Chord (BAC) using the peak width and the BRV as per Equation (34).
Once the BAC was obtained for all released bubbles, the bubble volume for each bubble with its respective bubble volume deviation was calculated. It was found that this deviation grew with the bubble size, with larger bubbles providing a larger deviation. This was consistent with an increased bubble perturbation of the bubble adjacent dense phase. Due to this, an approach to establish a “peak dependant baseline” for each peak was considered, in the present study.

To accomplish this, the average of the entire signal record was calculated first. Then, its standard deviation ($\sigma_s$) was established and used as follows: a) Multiples of $\sigma_s$, from 0 to 4, were subtracted from the average signal value, as shown in Figure 6-4, b) The resulting modified baseline signal provided an average BAC, which was compared to the one from the theoretical model, as reported in Figure 6-5.

Figure 6-4. Typical Peak Signal Showing the Influence of Different Selected Baseline on the Peak Width.

Figure 6-5a) and b) report the $\sigma_s$ Baseline Modifier (BLM) as a function of the measured BAC. Figure 6-5a) shows $\sigma_s$ Baseline Modifier in the 0 to 4 range and how these BLM values reduce the average measured Bubble Axial Chords. Thus, an optimization of $\sigma_s$ modifiers allows
calculating the bubble injected volume with a 4% average error, and with all the BLM modifiers falling in the 0-1 range.

An explanation of this method is provided in Figure 6-5b). Given that the predicted BAC from Model #2 (black squares) and the predicted BAC for different BLM modifiers, one can see that their intersection provides the advised BLM. For instance, for a) Bubbles with a 0.105 m non-treated BAC (NTBAC), the BLM was set at 0.94, b) Bubbles with a 0.087 m NTBAC, the selected BLM was 0.75, c) Bubbles with a 0.075 m NTBAC, the chosen BLM was 0.05, d) Bubbles with NTBACs smaller than 0.073 m, the BLM was set at zero.

![Figure 6-5. a) Average BAC of each Data Series with a Baseline at Different Signal Heights, Compared with the Theoretical Model BAC Size of each Data Series. b) Expanded Detail for the Range from 0 to 1 BLM. The green area represents the amount of correction needed for each BAC.](image)

One should note that the proposed method of calculation allows one to make interpolated BAC corrections with bubbles generated in the 138 to 345 kPa range, as described in Figure 6-5(b). Using the described method, all-raw CREC Optiprobe signals were re-analyzed for each bubble peak.
Bubble motion in a fluidized bed is a process that intrinsically contains randomness. This randomness generates few outliers. After the bubble peak treatment, these few outliers (e.g., close to 10% of all data collected) were eliminated from the BAC data pool. This approach consisted of first establishing a normal data distribution. Following this, the distribution of the first and third quartiles was determined. Then, 1.5 times of the first and third quartile difference were subtracted and added respectively to 25% and 75% of the area distribution. Once this process was complete, all data points outside this normal distribution range were designated as outliers and eliminated from further data treatment.

Furthermore, once the optimum $\sigma_s$ multiple for every condition was defined, the height of the baseline was calculated as per Equation (51) as follows:

$$h_{bl} = \frac{\sum_1^n (Voltage \, Signal)_n}{n} - BLM \times \sigma_s$$  \hspace{1cm} (51)

One should note that the effect of using $\sigma_s$ baseline bubbles multipliers (BLM), on the Bubble Rise Velocity (BRV) is negligible, since the BRV velocities remain essentially constant, regardless of the BLM assigned as shown in Figure 6-6.
Figure 6-6. Average Bubble Rise Velocity (BRV), for Different BLMs to Determine the Effect of the Influence of Data Processing on the BRV.

6.2 Secondary Bubble Detection

Signals obtained by the CREC-Optiprobes showed in some cases a higher BRV than expected, and this was as predicted by Eq. 29. This happened to approximately 5% of all bubbles recorded. These bubbles displayed CREC Optiprobes signal double peaks and were carefully re-examined.

Figure 6-7 reports a schematic description of a CREC Optiprobes signal doublets, with a leading bubble followed by a secondary smaller bubble.
This bubble configuration, consisting of a pair of close bubbles, was observed mainly for 345 and 414 kPa injection pressures and was assigned to an inherent failure when injecting single bubbles at higher injection pressures. Bubbles recorded that presented this higher BRV were accounted for in our calculation methodology, as single bubbles with a volume equal to the sum of the volume of the two close bubbles in the train.
6.3 Conclusions

a) Data voltage sets obtained using the CREC Optiprobes require a baseline setting with bigger bubbles requiring a more significant baseline correction.

b) Peak baseline adjustment involves the use of the HESC model, with an assumed bubble shape, as described in Chapter 5.

c) Images of the frontal radius of the bubble taken by the video camera need to be processed to transform the number of pixels in the bubble frontal radius image into a measurement in cm.
Chapter 7: **Experimental Data Results and Discussion**

### 7.1 Application of the Proposed HESC Model

The proposed HESC Model requires validation. In this respect, one can consider a single bubble injected into a sand bed at minimum fluidization without biomass pellets loaded in the bed. Given that, in principle, there should be the same air moles injected bubble and measured bubble in the bed, at various axial positions, and assuming that the ideal gas law can be applied, one can arrive at the following:

\[
N_{inj} = \frac{P_{inj}V_{inj}}{RT} = N_{bubble} = \frac{P_{bubble}V_{bubble}}{RT} \tag{52}
\]

With \(P_{inj}\) and \(V_{inj}\) representing the pressure and volume of the bubble injected, \(P_{bubble}\) and \(V_{bubble}\) describing the pressure and volume of bubble inside the bed, \(T\) representing the temperature in degrees Kelvin and \(R\) denoting the universal gas constant.

Given that under these conditions, the temperature of the injected bubble and that of the bubble in the bed are constant, Equation (53) can be reduced to:

\[
V_{cylinder}P_{cylinder} = V_{bubble}P_{bed-surface} \tag{53}
\]

With the total pressure at the bed surface (\(P_{bed-surface}\)) being set to 1.05 atm (106.8 kPa).

One should mention that Equation (53) does not include an eventual gas exchange between the dense and the diluted phases in the bed. This assumption is based on the work of Kunii and Levenspiel (Kunii and Levenspiel, 1968), where it is stated that the main cause behind the gas interchange between phases is the excess of airflow above the minimum fluidization velocity. Since the present model validation was carried out with the bed of sand at minimum fluidization...
velocity \( U_{mf} = 0.17 \text{ m/s} \), it is possible to assume with confidence that such a phase interchange is negligible.

However, and to fully confirm this assumption, volume balances based on measured and predicted bubble volumes were made, differing from each other, about 9% on average. Thus, once the volume of injected air was established, the volume of the wake, the total volume of the sphere, the bubble radius, and the Bubble Axial Chord (BAC) were assessed using Equations (36) to (39), (44) and (45). The results of these calculations are reported in Table 7-1.

Table 7-1. Theoretical BAC Model Results as per Equations (36) to (38), and Equation (39) for Model 1, and Equation (50) for Model 2.

<table>
<thead>
<tr>
<th>Manometric Pressure at Cylinder (kPa)</th>
<th>Air Volume injected ( V_b ) (10(^6)m(^3))</th>
<th>Wake Volume ( V_w ) (10(^6)m(^3))</th>
<th>Total Volume ( V_T ) (10(^6)m(^3))</th>
<th>Sphere Radius, ( R ) (m)</th>
<th>BAC (m)</th>
<th>Deviation between Models</th>
</tr>
</thead>
<tbody>
<tr>
<td>138</td>
<td>336</td>
<td>87</td>
<td>423</td>
<td>0.046</td>
<td>0.067</td>
<td>0.068</td>
</tr>
<tr>
<td>207</td>
<td>433</td>
<td>112</td>
<td>545</td>
<td>0.051</td>
<td>0.073</td>
<td>0.074</td>
</tr>
<tr>
<td>276</td>
<td>529</td>
<td>138</td>
<td>667</td>
<td>0.054</td>
<td>0.078</td>
<td>0.080</td>
</tr>
<tr>
<td>345</td>
<td>626</td>
<td>163</td>
<td>789</td>
<td>0.057</td>
<td>0.082</td>
<td>0.084</td>
</tr>
</tbody>
</table>

One can notice that both Model 1 (spherical bubble cap with flat interface) and Model 2 (spherical bubble cap with waving interface) provide close BACs, increasing consistently with the injection pressure and having deviations smaller than 2%. These BAC theoretical derived values for both Model 1 (Equation (39)) and Model 2 (Equation (50)) will be used later in the present study to compare them with BAC experimental data.
7.1.1 Application of the BAC Data Treatment

Table 7-2 reports the BACs (NTBACs) as directly obtained from experiments with no correction of the baseline. As a result, the reported NTBAC values provide a starting point for data treatment.

Table 7-2. Values of Pre-treatment BACs Compared to Theoretical Values.

<table>
<thead>
<tr>
<th>Pressure of injection (kPa)</th>
<th>Non-Treated BAC (NTBAC) (m)</th>
<th>Model #2 BAC (m)</th>
<th>Bubbles analyzed</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Average</td>
<td>St. Dev.</td>
<td></td>
</tr>
<tr>
<td>138</td>
<td>0.069</td>
<td>43%</td>
<td>0.068</td>
</tr>
<tr>
<td>207</td>
<td>0.081</td>
<td>45%</td>
<td>0.074</td>
</tr>
<tr>
<td>276</td>
<td>0.091</td>
<td>44%</td>
<td>0.080</td>
</tr>
<tr>
<td>345</td>
<td>0.147</td>
<td>93%</td>
<td>0.084</td>
</tr>
</tbody>
</table>

The values reported in Table 7-2 show that the raw measured BAC data, obtained with the CREC Optiprobe system before data treatment, is significantly different than those of model predictions, having a high standard deviation of up to 93%.

Thus, the various statistical parameters considered display significant deviations with the RMSE and BIAS reaching 14.72 and -6.25, respectively, for a 345 kPa, as one can notice in Table 7-6. Furthermore, the MRAE ranges from 22% to 88% for all the injected pressure values.
Figure 7-1 reports the distribution of Non-Treated BACs (NTBAC) for the injected bubbles at various air pressures. Reported boxes contain 25%-75% BAC distribution data, which suggests an increased standard deviation, as reported in Table 7-2, for bubbles injected at increased pressures. Thus, and on this basis, a further data analysis using the non-treated BACs, including outlier removal, is advised, as described in Section 6.1. Table 7-3 reports the results of such analysis.

**Table 7-3. Values of Treated BACs Compared to Theoretical Values.**

<table>
<thead>
<tr>
<th>Pressure of injection (kPa)</th>
<th>BAC (m)</th>
<th>Model #2 BAC (m)</th>
<th>Bubbles analyzed</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Average</td>
<td>St. Dev.</td>
<td></td>
</tr>
<tr>
<td>138</td>
<td>0.068</td>
<td>17%</td>
<td>0.068</td>
</tr>
<tr>
<td>207</td>
<td>0.074</td>
<td>17%</td>
<td>0.074</td>
</tr>
<tr>
<td>276</td>
<td>0.077</td>
<td>22%</td>
<td>0.080</td>
</tr>
<tr>
<td>345</td>
<td>0.087</td>
<td>27%</td>
<td>0.084</td>
</tr>
</tbody>
</table>

One can see in Table 7-3 that the experimental data after treatment is closer to the simulation model predicted values. In addition, when comparing this with the values reported in Table 7-2, one can notice that there is a significantly reduced standard deviation. Additional
statistical error indicators, as reported in Table 7-7, confirm the same trends when compared to Table 7-6.

Figure 7-2 describes both the distribution of the resulting BACs, using boxes containing from 25%-75% of the revised BAC distribution. Furthermore, plot whiskers contain 1.5 of the BAC distribution interquartile range. Thus, and on this basis, one can see the major beneficial effect of the proposed baseline setting process.

Furthermore, when comparing Figure 7-2 and Figure 7-1, it becomes apparent that the mean and the median for each series display close values, data dispersions are smaller, and the expected BAC increase with an injected air volume is better predicted. As well, the resulting more symmetrical BAC distribution supports the assigned BAC normal distribution, when later in the Ph.D. Dissertation, one develops standard deviation analysis and deletes outliers from further consideration.

Thus, as shown in Figure 7-2, it was proven that the proposed baseline correction methodology is effective, reducing the error on the experimentally measured BACs.
7.1.2 Frontal Bubble Radius

Regarding the fluidized bed unit, it was operated at minimum fluidization velocity to avoid that additional bubbles be formed in addition to the ones injected. Regarding bubbles injected, their size was changed by feeding air at various pressures into the injection chamber. The pressures used were 138 kPa, 207 kPa, 276 kPa, and 345 kPa. Thus, as bubbles were produced with the as shown in Figure 4-8, the video camera recorded injected bubbles at the bed surface.

The analysis of the video images was achieved by dividing the images into frames, with each second of video providing 30 frames or still images. Each video frame was inspected to find a bubble. When a bubble was found, the number of pixels of its radius was recorded. This was done for every single bubble observed and for all frames recorded. Furthermore, using the diameter of the bed as a reference, the pixels were assigned dimensions in centimeters.

Concerning the recorded frames for every bubble, they are reported in Figure 7-3(a), Figure 7-3(b), Figure 7-3(c), and Figure 7-3(d) for the four air pressures used to fill the air-pressurized bottle. It was observed that in all cases, when analyzing consecutive frames, the frontal bubble radius increased until a maximum value was reached. Following this, the frontal bubble radius decreased progressively until the value of zero was attained. This occurred when the bubble left the bed. One can observe in this respect, that while for the 138 kPa injection pressure the maximum frontal bubble radius was observed in the third frame, for both the 207 kPa and 276 kPa injection pressures, the maximum frontal bubble radius was observed in the fourth frame. Furthermore, for the 345 kPa injection pressure, the maximum value was recorded in the 7th frame. It should be noticed that these findings are consistent with larger injection pressures, forming bigger bubbles and consequently bubbles with a larger frontal bubble radius.
Figure 7-3. Changes of the Bubble Frontal Radius over Time as Recorded with the Video Camera. Bubble are injected under the following conditions: a) 138 kPa, b) 207 kPa, c) 276 kPa, and c) 345 kPa.

Table 7-4 reports a comparison of the theoretical predicted frontal radius (Equation (38)) and the experimentally obtained ones. This frontal bubble radius is calculated using the extrapolated R-value at the hypothetical number of zero frames, as shown in Figure 7-3(a), Figure 7-3(b), Figure 7-3(c), and Figure 7-3(d). One can observe that the average deviation between the theoretical model and experimental observations remains below 6%, which provides validation to the methodology proposed in the present study.
Table 7-4. Comparison Between Theoretical and a Measured Frontal Bubble Radii in a Sand Fluidized Bed.

<table>
<thead>
<tr>
<th>Pressure Of injection (kPa)</th>
<th>The volume of Injected air (10^6 m^3)</th>
<th>“Frame Zero” Size (m)</th>
<th>Theoretical Radius (m)</th>
<th>Number of Frames Considered</th>
<th>Deviation from Model #2</th>
</tr>
</thead>
<tbody>
<tr>
<td>138</td>
<td>354.1</td>
<td>0.048±0.0033</td>
<td>0.046</td>
<td>96</td>
<td>2%</td>
</tr>
<tr>
<td>207</td>
<td>456.2</td>
<td>0.055±0.0074</td>
<td>0.051</td>
<td>105</td>
<td>6%</td>
</tr>
<tr>
<td>276</td>
<td>558.2</td>
<td>0.056±0.0082</td>
<td>0.054</td>
<td>84</td>
<td>1%</td>
</tr>
<tr>
<td>345</td>
<td>660.3</td>
<td>0.060±0.0069</td>
<td>0.057</td>
<td>204</td>
<td>3%</td>
</tr>
</tbody>
</table>

Thus, and on this basis, one can conclude that the combined application of the CREC Optiprobies and the video camera, as attempted in the present study, leads to an adequate measurement of both the frontal bubble radius and the BAC.

7.2 Discussion of Results

7.2.1 Bubble Axial Chord (BAC) in a Sand Fluidized Bed Loaded with Biomass Pellets

Figure 7-4 illustrates the biomass addition effect. This shows that both the BAC size and the BRV are reduced, and this once the analog biomass pellets are introduced in the bed, with this effect increasing at higher biomass concentrations.
Figure 7-4. Average BAC Changes for Each Series of Bubbles with Biomass Content (vol%). For every point reported in this plot, between 18 and 73 bubbles were considered.

Regarding the statistical error parameters, they significantly increase in all cases, for both 5 vol% and 10 vol% of analog biomass pellets loadings. Thus, this means that biomass addition, while reducing the average BAC, leads to a wide BAC distribution, with this being assigned to the intrinsic nature of the analog biomass pellet effect on bubble breaking. Detailed information regarding this statistical error parameters is given in Table 7-8.
7.2.2 Single Bubble Velocity in a Sand Fluidized Bed Free of Biomass Pellets

Figure 7-5 reports that BRV increases with BAC in a fluidized bed free of biomass pellets.

![Figure 7-5. Correlations Between BRV and BAC Compared to Experimental Results Obtained in the Absence of Biomass Pellets.](image)

While Figure 7-5 reports an increasing BRV with BAC. To show that this is in line with previous studies that $d_{beq}$ instead of the BAC as the characteristic bubble dimension, the geometrically based Equation (54) was used.

$$BAC = \beta_0 d_{beq}$$

with $\beta_0 = 0.7791$ was considered.

Figure 7-5 also shows that the bubble velocity appears for a 0.04-0.12 m BAC-size bubbles in the 0.5 to 1.4 m/s range. This influence of BAC on BRV should be considered as a probabilistic BRV phenomenon, with BRV varying significantly for a set BAC value. These experimental results also show that the BRV does not stabilize for larger BACs, as predicted by various models reported in Figure 7-5.
7.2.3 Single Bubble Velocity in a Sand Fluidized Bed Loaded with Biomass Pellets

Furthermore, and to consider the biomass pellets' effect on the BRV, biomass pellets were added to a fluidized bed under incipient fluidization conditions. Single bubble experiments were repeated as described in Section 4.1, with 5 vol% and 10 vol% biomass pellets being added into the bed. The sand bed operated at 0.17 m/s minimum fluidization for conditions of operation with and without pellets. As well, bubbles were generated using 138 kPa, 207 kPa, 276 kPa, 345 kPa, and 414 kPa in the air-pressurized bottle.

Figure 7-6 reports the BRV at various BACs for pressures of injection of (a) 138 kPa, (b) 207 kPa, (c) 276 kPa, (d) 345 kPa and (e) 414 kPa with different biomass contents, from 0 vol% to 10 vol%.

Figure 7-6(a), describes the experimentally observed BRVs and BACs for a 138 kPa injection pressure at 5 vol% and 0 vol% biomass concentrations. One can thus see that as the sand bed is loaded with biomass particles, there is a significant reduction of both BACs and BRVs. For instance, for a bubble injected without biomass, an average 0.067 m BAC was observed, while with 5 vol% of biomass, a 0.03m average BAC was recorded. As well, it is possible to notice that, given BRVs change in BAC ranges, with this variation being assigned to the probabilistic nature of rising bubbles.
Figure 7-6. BRV vs. BAC for Different Sizes of Bubbles Injected with Different Concentrations of Biomass: a) 138 kPa, b) 207 kPa, c) 276 kPa, d) 345 kPa, e) 414 kPa were used to inject the bubble.
Furthermore, Figure 7-6(b), Figure 7-6(c), Figure 7-6(d), and Figure 7-6(e) compare bubbles in sand fluidized beds without free of biomass at various injection pressures. One can also observe bubbles BACs and BRV when 5 vol% and 10 vol% of biomass pellets were added at 207 kPa, 276 kPa, 345 kPa, and 414 kPa of injection pressure. One can notice that in all cases, there is an important reduction of BACs and BRVs. For instance, in Figure 7-6(b) at 207 kPa of injected air pressure, it is shown that the average BAC for the bed free of biomass is close to 0.08 m. However, when 5 vol% is added to the bed, the average BAC value becomes 0.06 m. With 10 vol% biomass, the average BAC is reduced further to 0.04 m. As well, the BRV values decrease when adding biomass from 0.8 m/s to 0.6 m/s and to 0.3 m/s, respectively.

Similar results are reported in Figure 7-6(c) with 276 kPa of air bubble injection pressure. Average BACs of 0.085 m with 0.9 m/s BRV decrease to 0.06 m with 5 vol% of biomass, having a 0.5 m/s average BRV. Furthermore, by adding 10 vol% biomass, the average BAC becomes 0.04 m, and the average BRV becomes 0.35 m/s.

Figure 7-6(d) and Figure 7-6(e) describe bubble injection pressures of 345 kPa and 414 kPa with 5 vol% and 10 vol% biomass in the bed. In these cases, the major influence of biomass diminishes both BAC and BRV.

Regarding the BACs and BRVs observed experimentally, as shown in Figure 7-6(a), Figure 7-6(b), Figure 7-6(c), Figure 7-6(d) and Figure 7-6(e), one can notice that obtained data are distributed in a range delimited by the available models described in Section 2.1. Thus, available models do not predict well single bubbles dynamics evolving in sand fluidized beds without biomass. Due to their lack of accuracy, a modification to the empirical model originally proposed by Davidson and Harrison (Davidson and Harrison, 1963) is proposed here as follows.
\[ BRV = \gamma \sqrt{g \cdot BAC} \]  

(55)

where \( \gamma \) has a value of \( 0.86 \pm 0.00975 \) for the studied operational conditions.

One should mention that the postulated Equation (55) was obtained once unexpectedly fast bubbles were removed from the analysis. These bubbles with high BRVs are considered the result of bubble splitting, as described in Section 6.2. Thus, after removing these fast bubbles, the proposed model as per Equation (55) is shown in Figure 7-7.

Figure 7-7 also reports the recorded bubble data in the presence of biomass pellets and after removing the few outliers and double bubbles.
7.2.4 Evaluation of BAC Data Distribution

In order to assess the nature of the BAC data distribution, all runs were tested using the probabilistic plots of Figure 7-8. As can be seen, reported values fall in the 95% confidence interval of the 45 degrees line, in all cases. Thus, a normal BAC distribution can be considered in all experimental BAC data series, with and without biomass pellets.

Figure 7-9 also shows the BAC distribution for each run at various air pressure injections. Plots in the first column describe experiments carried out without biomass. Plots in the second column represent runs with 5 vol% biomass. Plots in the third column show experiments with 10 vol% biomass. On the other hand, rows in this figure describe BAC distributions at various air injection pressures of 138 kPa, 207 kPa, 276 kPa, 345 kPa, and 414 kPa.

Regarding Figure 7-9, one can notice the close to normal BAC distribution, which is always shifting towards lower BAC values, once the biomass pellets are loaded in the bed of sand. It is shown that for all runs, consistent normal BAC distributions were recorded.
Figure 7-8. Probability Plots for all the BAC Series that Show their Normal Distribution. Columns Represent Biomass Contents in vol% while Rows Represent Air Injection Pressure in kPa.
<table>
<thead>
<tr>
<th></th>
<th>0 vol%</th>
<th>5 vol%</th>
<th>10 vol%</th>
</tr>
</thead>
<tbody>
<tr>
<td>138 kPa</td>
<td><img src="image1" alt="Histogram" /></td>
<td><img src="image2" alt="Histogram" /></td>
<td><img src="image3" alt="Histogram" /></td>
</tr>
<tr>
<td>207 kPa</td>
<td><img src="image4" alt="Histogram" /></td>
<td><img src="image5" alt="Histogram" /></td>
<td><img src="image6" alt="Histogram" /></td>
</tr>
<tr>
<td>276 kPa</td>
<td><img src="image7" alt="Histogram" /></td>
<td><img src="image8" alt="Histogram" /></td>
<td><img src="image9" alt="Histogram" /></td>
</tr>
<tr>
<td>345 kPa</td>
<td><img src="image10" alt="Histogram" /></td>
<td><img src="image11" alt="Histogram" /></td>
<td><img src="image12" alt="Histogram" /></td>
</tr>
<tr>
<td>414 kPa</td>
<td><img src="image13" alt="Histogram" /></td>
<td><img src="image14" alt="Histogram" /></td>
<td><img src="image15" alt="Histogram" /></td>
</tr>
</tbody>
</table>

*Figure 7-9. Histogram for each BAC Data Series. Columns Represent Biomass Contents in vol% while Rows Represent Air Injection Pressure in kPa.*
7.2.5 Statistical Analysis

The present statistical analysis section reports the various error parameters applied to the data sets. These considered parameters allow to visualize the deviation from models, the dispersion of measurements, and the over or under prediction trends.

Data obtained through the experiments were compared with the theoretical predictions of Model #2 (Equation (50)) and the data treatment method using the following statistical error parameters as reported in Table 7-5.

*Table 7-5. Equations for the Statistical Error Parameters Used in this Study.*

<table>
<thead>
<tr>
<th>Name</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Root Mean Squared Error</td>
<td>( \text{RMSE} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (f_i - y_i)^2} )</td>
</tr>
<tr>
<td>(RMSE)</td>
<td>(56)</td>
</tr>
<tr>
<td>Mean Signed Error</td>
<td>( \text{BIAS} = \frac{1}{n} \sum_{i=1}^{n} (f_i - y_i) )</td>
</tr>
<tr>
<td>(BIAS)</td>
<td>(57)</td>
</tr>
<tr>
<td>Mean Relative Absolute Error</td>
<td>( \text{MRAE} = \frac{1}{n} \sum_{i=1}^{n} \left</td>
</tr>
<tr>
<td>(MRAE)</td>
<td>(58)</td>
</tr>
<tr>
<td>Mean Relative Signed Error</td>
<td>( \text{MRSE} = \frac{1}{n} \sum_{i=1}^{n} \left( \frac{f_i - y_i}{f_i} \right) )</td>
</tr>
<tr>
<td>(MRSE)</td>
<td>(59)</td>
</tr>
<tr>
<td>Standard Error</td>
<td>( \text{SE} = \frac{\sigma}{\sqrt{n}} )</td>
</tr>
<tr>
<td>(SE)</td>
<td>(60)</td>
</tr>
</tbody>
</table>

Table 7-5 reports a statistical error analysis of various NTBACs. This is prior to the more detailed BAC correction, as described in Section 4.1. Statistical error parameters used in this table are as follows: a) Root Mean Squared Error (RMSE), b) Mean Signed Error (BIAS), c) Mean Relative Absolute Error (MRAE), d) Mean Relative Signed Error (MRSE) and e) Standard error (SE). In this regard, RMSE and BIAS values are useful to compare sets of data, in this case, before
data treatment, and after data treatment. The RMSE relies on both the magnitude and the dispersion of the set of data, while the BIAS gives information about consistent model underestimation or overestimation. Relative MRAE and MRSE error indicators provide additional model viability evaluation.

Table 7-6. Statistical Error Parameters of Experimentally Measured NTBACs as Compared to the Theoretical Value Calculated from the Proposed Model #2.

<table>
<thead>
<tr>
<th>Pressure of injection (kPa)</th>
<th>Statistical Error Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>RMSE</td>
</tr>
<tr>
<td>138</td>
<td>2.93</td>
</tr>
<tr>
<td>207</td>
<td>3.65</td>
</tr>
<tr>
<td>276</td>
<td>4.13</td>
</tr>
<tr>
<td>345</td>
<td>14.72</td>
</tr>
</tbody>
</table>

Table 7-6 shows the various RMSE, BIAS, MRAE, MRSE, and SE statistical error parameters. This table reports a significant decrement in the size of all the maximum BIAS and RMSE error indicator values, from 14.72 to 2.29 and from -6.25 to 0.30, respectively. As well, maximum MRAE and MRSE relative indicator errors are now being diminished from 0.88 to 0.23 and from -0.74 to -0.04.

Table 7-7. Statistical Error Parameters for the Experimentally Measured BAC After the Data Treatment Process Compared to the Theoretical Values Calculated from the Proposed Model #2.

<table>
<thead>
<tr>
<th>The pressure of injection (kPa)</th>
<th>Statistical Error Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>RMSE</td>
</tr>
<tr>
<td>138</td>
<td>1.10</td>
</tr>
<tr>
<td>207</td>
<td>1.20</td>
</tr>
<tr>
<td>276</td>
<td>1.68</td>
</tr>
<tr>
<td>345</td>
<td>2.29</td>
</tr>
</tbody>
</table>
Table 7-7 reports statistical error parameters for all the experimental data obtained with and without added biomass, using as the basis of the analysis the RMSE, the BIAS, the MRAE, the MRSE, and the SE, as defined in Table 7-5. Table 7-8 shows that in all cases, the various statistical parameters are significantly increased, with this being the case for both 5 vol% and 10 vol% of biomass pellets loadings. Thus, this means that biomass addition, while reducing the average BAC, leads to a wide BAC distribution, with this being assigned to the intrinsic nature of the biomass pellet effect on bubble breaking.

Table 7-8. Statistical Error Parameters for the BAC Measured in the Presence of Biomass Inside the Reactor.

<table>
<thead>
<tr>
<th>The pressure of injection (kPa)</th>
<th>BM vol%</th>
<th>Statistical Error Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>RMSE</td>
</tr>
<tr>
<td>138</td>
<td>0</td>
<td>1.10</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>4.21</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>2.29</td>
</tr>
<tr>
<td>207</td>
<td>0</td>
<td>1.20</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>3.75</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>2.12</td>
</tr>
<tr>
<td>276</td>
<td>0</td>
<td>1.68</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>3.90</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>2.76</td>
</tr>
<tr>
<td>345</td>
<td>0</td>
<td>2.29</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>3.67</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>1.80</td>
</tr>
<tr>
<td>414</td>
<td>5</td>
<td>3.41</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>2.46</td>
</tr>
</tbody>
</table>
7.3 Conclusions

a) Biomass analog pellets have a significant influence on reducing both the BAC and the BRV.

b) Biomass pellets act as bubble breakers in the sand bed at incipient fluidization conditions.

c) Biomass pellets contribute to having both a normal and wider BAC distribution.

d) The $BRV = \gamma \sqrt{g \cdot BAC}$ equation for bubbles in sand fluidized beds without biomass can also be extended when biomass pellets are added to the bed.

e) The $BRV = \gamma \sqrt{g \cdot BAC}$ derived equation provides a framework for establishing consistency between BRV and BAC numerical calculated values.
Chapter 8: CFD-MPPIC Modeling of single bubbles

After developing the experimental methodology to obtain and process bubble size, bubble shape, and bubble velocity data for single bubbles, by combining the CREC Optiprobe system and the video camera, the obtained results were compared to the HESC model. This created a shape reference for the experimental bubbles in order to determine measurement accuracy. Thus, experimental data agreement with the mathematical model was considered a validation of both the proposed model and the experimental method.

In this regard, a simulation of the single bubble dynamics was considered to provide another layer of validation to the experimental data and to help consolidate a set of input parameters that will allow one to replicate the experiments numerically. This is considered very valuable for further fluidized bed gasifier unit scaling, incorporating both kinetics and energy balances in the calculations.

Due to the many advantages of the CFD-MPPIC method, described in Section 2.2, it was chosen to simulate the single bubble dynamics numerically. One should notice that, although the selected methodology states that there is no change in particle mass or mass transfer between the phases, during the gasification process, the biomass particles are consumed and transformed. This difference can be resolved by the assumption of a constant biomass feed that compensates the biomass consumption, yielding a steady mass following the methodology assumptions.

This chapter expands on the details of how the input parameters of the model were selected and what tests were performed to ensure the validity of the numerical simulations.
8.1 Initial, boundary conditions, and convergence criteria.

During the CFD-MPPIC simulations developed to determine the adequate parameters to use in the numerical calculations of the gasifier cold-model, the same initial and boundary conditions were applied.

8.1.1 Initial conditions

There were two types of initial conditions (IC) applied to all simulations in this study: a) fluid IC, and b) particle IC. The fluid initial condition was defined with air being at rest (0 m/s), 300 K, and 101325 Pa (1 atm). Regarding the particle IC, there were two, one for the sand and one for the biomass. Both of them were defined considering the material properties, their total mass, and the geometrical space they occupied. The sand was defined with 109 kg for all simulations, in a bed occupying between 0 m to 0.45 m column height. One should note that the mass value assigned to the sand as IC is consistent with experimental measurements effected in the gasifier cold model. On the other hand, biomass was defined with 0.648 kg or 1.296 kg for 5 vol% and 10 vol% loadings, respectively, placed in the same column section as for the sand particles. This region was, however, taller than the bed observed in the experimental setup, and this to allowed the sand and biomass to fall and settle down on the first iteration of the CFD-MPPIC numerical simulations.

8.1.2 Boundary conditions

There were three types of boundary conditions (BC) in all the numerical calculations of this study: a) Pressure BC, b) Flow BC, and c) Injection BC.

The Pressure Boundary Condition (PBC) refers to the pressure outlet of the gasifier cold model, which was defined at column top using as a flat disc containing all cells adjacent to the top
border of the geometry. This Pressure BC was defined as “open to the atmosphere,” which means it has a pressure of 101325 Pa, and it does not allow transit of particles through it.

Regarding the *Flow Boundary Condition (FBC)*, it defines the airflow through the distributor into the column. This flow was defined as a disc made by cells at the bottom of the grid. This BC was set differently for different simulations. In the case of the grid evaluation calculations, a slope of increasing velocity was used, followed by a slope of decreasing velocity, in agreement with the experiment considered. For all other simulations, a fixed value of 0.20 kg/s was set. This value corresponds to the “incipient fluidization” regime as explained before, in this regime, the sand is almost at the fluidization point but it does not generate other bubbles.

The *Injection Boundary Condition (IBC)* is the one that replicated the bubble injection, as described in Section 4.6. This IBC was defined using nozzles location, the width of the nozzle, and mass flow injection profile. The IBC location for 0.004 m diameter nozzle was placed at the center of the column and 0.08 m above the distributor, and this to match the experimental setup configuration. The described mass flow injection profile was defined through an equation derived from the Bernoulli principle, as it is explained later in this chapter.

### 8.1.3 Convergence criteria

Throughout all the numerical calculations developed in the present study, the same convergence criteria were used. The number of iterations and size of residuals was set for volume, pressure, and velocity calculations, as shown in Table 8-1.
Table 8-1. Convergence criteria for all the simulations in this study

<table>
<thead>
<tr>
<th></th>
<th>Iterations</th>
<th>Residual</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume</td>
<td>10</td>
<td>1x10^-7</td>
</tr>
<tr>
<td>Pressure</td>
<td>2000</td>
<td>1x10^-6</td>
</tr>
<tr>
<td>Velocity</td>
<td>501</td>
<td>1x10^-7</td>
</tr>
</tbody>
</table>

The other factor considered for the convergence, accuracy, and stability of the calculations was the Courant–Friedrichs–Lewy Number (CFL Number). This number has to be maintained between 0.8 and 1.5 (CPFD Software LLC., 2019). The time step was chosen to be 0.001s, and this in order to allow the calculations to sustain this level of CFL Number, although Barracuda VR® can modify the timestep if necessary, to ensure this criterion is achieved.

8.2 Grid Independence Test

CPFD Barracuda VR® uses structured grids to make calculations. Working with the biggest grid possible without losing numerical result resolution is always a challenge in CFD. In particular, for the present study, where biomass pellets are added to a sand bed, the selection of the grid size is critical as cell sizes are always larger than the particle size.

Therefore, a test was performed using 4 different grids as follows: a) a coarse grid mesh with 11592 cells, having a 1.293x10^-5 m³ average volume and a 2.347x10^-2 m average length, b) a medium grid mesh with 41472 cells, having a 3.616x10^-6 m³ average volume and a 1.535x10^-2 m average length, c) a fine grid mesh with 107568 cells, having a 1.705x10^-6 m³ average volume and a 1.19460x10^-2 m average length, and d) a grid ultra-fine mesh with 141512 cells, having a 1.060x10^-6 m³ average volume and a 1.020x10^-2 m average length.

The bed was pre-fluidized with an air velocity of 0.10 m/s for a 10 seconds period. At the end of this time, the fluid velocity profile in the freeboard was recorded at 60 cm above the
distributor or 20 cm above the static bed surface. The 3D velocity profile for each grid is shown in Figure 8-1.

Figure 8-1 shows that the grid size of the mesh had an influence on the radial air velocity simulated. For example, the medium and fine grid meshes provided smoother profiles, with this being in contrast with the significant radial variations of the coarse grid mesh. On the other hand, while the ultra-fine grid displayed a slight improvement in the air velocity profile uniformity across the horizontal unit section, its high computational cost was especially noticed. As a result, the fine size grid was selected for further computations.
Figure 8-1. 3D Air Velocity Profile in the freeboard at 60 cm Above the Distributor Using: a) A coarse grid mesh with 11592 cells, an $1.293 \times 10^{-5}$ m$^3$ average volume and a $2.347 \times 10^{-2}$ m average length, b) A medium mesh with 41472 cells, a $3.616 \times 10^{-6}$ m$^3$ average volume, and a $1.535 \times 10^{-2}$ m average length, c) A fine mesh with 107568 cells, a $1.705 \times 10^{-6}$ m$^3$ average volume, and a $1.19460 \times 10^{-2}$ m average length d) An ultra-fine mesh with 141512 cells, a $1.060 \times 10^{-6}$ m$^3$ average volume, and a $1.020 \times 10^{-2}$ m average length.

8.3 Reproducibility of Results and Wall Effect Assessment

CPF-MPPIC simulations allow one to set two parameters for the wall momentum retention, the normal-to-wall momentum retention, and the tangential-to-wall momentum retention. These parameters can be set between 0 and 1, meaning no retention at all (total loss of momentum to the wall) or total momentum retention (elastic collision with the wall), respectively.

Thus, and to determine if there was a wall effect on single bubbles in a 3D sand fluidized bed, single bubbles with a volume of 433 cm$^3$ each were injected multiple times, changing at the
same time, the restitution coefficient at the wall as follows: 0 momentum retention, 0.5 momentum retention, and 1 momentum retention.

Figure 8-2 reports the result of the CFD-MPPIC simulations. One can see that due to their natural randomness, equal size bubbles injected at different times, are not identical or evolve in the same manner. Nevertheless, bubbles that have close size display a similar shape and growth, having almost identical rise velocities. Thus, one can conclude on this basis that the wall interaction with the bubbles does not affect single bubble rise velocities. This is given that all of the bubbles were detected at the same height at very similar times, with bubbles studied showing approximately the same BAC. In summary, the reported results support our study’s previous assumption that the single bubble dynamics is not affected by the unit walls, and that the results are highly reproducible.
Figure 8-2. CFD-MPPIC Simulation Progression of the Bubble 02 (433 cm3) as it Rises in the Reactor, with Different Wall Restitution Coefficients s follows a) 0 restitution coefficient, b) 0.5 restitution coefficient, c) 1 restitution coefficient.
8.4 Drag Model Selection Using Experimental Data

The drag model is significant in CFD-MPPIC simulations. As a result, various $C_D$ models described in Section 2.4 were examined on the basis of their ability to predict bed pressure drops at conditions close to minimum fluidization.

This pressure differential analysis involved an increasing air velocity from 0 m/s to 1 m/s in a 30 s period followed by a decreasing air velocity from 1 m/s to 0 m/s during 30 s. Pressure taps were located at 5 cm and 70 cm from the distributor. The lower tap was positioned in the dense bed while the higher tap was positioned in the freeboard.

According to the technical literature, when the airflow velocity increases (forward increase), the pressure differential augments up to a maximum value, due to the forces additional to gravity that the fluid has to transfer to the sand phase to unlock it from interparticle interactions before fluidization is achieved, before falling to a stable level at a slightly lower pressure differential. However, when the airflow velocity is reduced (backward reduction), the pressure differential stays at maximum pressure until the pressure starts to decrease at a rate similar to one observed in the forward direction (Kunii and Levenspiel, 1991).

Experiments were developed to establish these trends and to determine minimum fluidization velocity ($u_{mf}$) for the sand particles of the present study. Runs were performed using the experimental setup of Figure 4-1. This laboratory-scale unit includes a lower fluidized bed section with a 44 cm diameter and a 104 cm length as well as an upper freeboard section of 72 cm in diameter and 88 cm length. The static bed of sand particles has a height of 43 cm. Additional information about this experimental setup can be found in Torres Brauer et al. (Torres Brauer et al., 2020).
Table 8-2 reports the sand particle size distribution (PSD) measured using a Mastersizer 2000 Laser Diffraction Particle Size Analyzer.

Table 8-2. Particle Size Distribution (PSD) of the Simulated Sand (SiO2).

<table>
<thead>
<tr>
<th>%</th>
<th>Particle Diameter (μm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>257.65</td>
</tr>
<tr>
<td>1.74</td>
<td>295.83</td>
</tr>
<tr>
<td>5.87</td>
<td>339.65</td>
</tr>
<tr>
<td>13.85</td>
<td>389.97</td>
</tr>
<tr>
<td>26.13</td>
<td>447.75</td>
</tr>
<tr>
<td>41.91</td>
<td>514.09</td>
</tr>
<tr>
<td>59.32</td>
<td>590.25</td>
</tr>
<tr>
<td>76.17</td>
<td>677.70</td>
</tr>
<tr>
<td>90.33</td>
<td>778.10</td>
</tr>
<tr>
<td>100</td>
<td>893.38</td>
</tr>
</tbody>
</table>

In addition, the following conditions were selected for comparison, for each one of the CFD-MPPIC simulations runs. This was done to evaluate the most suitable drag model.
Table 8-3. Input Parameters for the CFD-MPPIC Simulation of the Pressure Differentials.

<table>
<thead>
<tr>
<th>Total Number of Cells</th>
<th>405132</th>
</tr>
</thead>
<tbody>
<tr>
<td>Real Number of Cells</td>
<td>217796</td>
</tr>
<tr>
<td>Average Volume of Cells</td>
<td>2.46E-6 m³</td>
</tr>
<tr>
<td>Thermal Settings</td>
<td>Isothermal Flow @ 300K</td>
</tr>
<tr>
<td>Base Materials</td>
<td>Air (default parameters), SiO₂ (with ρ=2650 kg/m³)</td>
</tr>
<tr>
<td>Close-Packed Volume Fraction</td>
<td>0.65</td>
</tr>
<tr>
<td>Maximum Momentum Redirection from Collision</td>
<td>40%</td>
</tr>
<tr>
<td>Normal to Wall Momentum Retention</td>
<td>0.8</td>
</tr>
<tr>
<td>Tangent to Wall Momentum Retention</td>
<td>0.9</td>
</tr>
<tr>
<td>Diffuse Bounce</td>
<td>0</td>
</tr>
<tr>
<td>Particle Sphericity</td>
<td>0.86</td>
</tr>
<tr>
<td>P, β, ε (From stress model)</td>
<td>1 Pa, 3, 10-8 (respectively)</td>
</tr>
<tr>
<td>Timestep</td>
<td>0.001 s</td>
</tr>
<tr>
<td>Inlet Boundary Condition</td>
<td>Constant Slope from 0 to 1m/s in 30 s and Back for a 60 s Total.</td>
</tr>
<tr>
<td>Outlet Boundary Condition</td>
<td>Open to Atmosphere</td>
</tr>
<tr>
<td>c₁ and d₁ Parameters for Parameterized Syamlal O’Brien Drag Model</td>
<td>c₁=0.547, d₁=4.9972</td>
</tr>
</tbody>
</table>

Regarding the potential drag models available, they yielded, as shown in Figure 8-4, different minimum fluidization velocities. Since the selected drag model for CFD-MPPIC simulations, should be the one providing a \( u_{mf} \) in close agreement with experimental values, this condition was adopted as the first drag model selection criterion.
Figure 8-4. a) Comparison of $\Delta P$ changes with superficial gas velocity, as predicted by the Wen Yu-Ergun Model (Equation (11)), the Turton-Levenspiel Model (Equation (12)), the Syamlal-O’Brien Model (Equation (13)), and the Non-Spherical Ganser Model (Equation (16)), with experimental data. b) Comparison of $\Delta P$ changes with superficial gas velocity as predicted by the Parameterized Syamlal O’Brien Model (Equation (18)) and EMMS-Yang Model (Equation (30)). The blue dotted line in Figures 2a) and 2b) represents the $\Delta P$ experimental data.

Figure 8-4a) and Figure 8-4b) display the simulated $\Delta P$ using various Drag Models described in Section 2.4. One can see that the four models reported in Figure 8-4a) significantly diverge from the experimental data. On the other hand, in Figure 8-4b), one can observe that both the Syamlal O’Brien and the EMMS-Yang Methods provide a close matching of the measured $\Delta P$s. The approach from the Syamlal O’Brien Model is the preferred one for further studies, given its ability to be implemented with less involved computations.

8.5 CFD-MPPIC Simulation of Single Bubbles

8.5.1 Simulation Setup

Once the drag model and the grid configuration were selected, the simulation of the single bubble was performed. With this objective in mind, the following conditions were applied in CPFD Barracuda VR® (Table 8-4).
Table 8-4. Input Parameters Used on CPFD Barracuda VR® to Simulate Single Bubbles.

<table>
<thead>
<tr>
<th>Total Number of Cells</th>
<th>107568</th>
</tr>
</thead>
<tbody>
<tr>
<td>Real Number of Cells</td>
<td>87980</td>
</tr>
<tr>
<td>Average Volume of Cells</td>
<td>1.705e-6 m³</td>
</tr>
<tr>
<td>Thermal Settings</td>
<td>Isothermal Flow @ 300K</td>
</tr>
<tr>
<td>Base Materials</td>
<td>Air (default parameters), SiO₂ (with ρ=2650 kg/m³)</td>
</tr>
<tr>
<td>Close-Packed Volume Fraction</td>
<td>0.635</td>
</tr>
<tr>
<td>Maximum Momentum Redirection from Collision</td>
<td>40%</td>
</tr>
<tr>
<td>Normal to Wall Momentum Retention</td>
<td>0.85</td>
</tr>
<tr>
<td>Tangent to Wall Momentum Retention</td>
<td>0.85</td>
</tr>
<tr>
<td>Diffuse Bounce</td>
<td>0</td>
</tr>
<tr>
<td>P, β, ε (From stress model)</td>
<td>1 Pa, 3, 10-8 (respectively)</td>
</tr>
<tr>
<td>Timestep</td>
<td>0.001 s</td>
</tr>
<tr>
<td>Outlet Boundary Condition</td>
<td>Open to Atmosphere</td>
</tr>
<tr>
<td>Air Mass Flow at Inlet</td>
<td>0.020 kg/s</td>
</tr>
</tbody>
</table>

Regarding the particles used in this CFD-MPPIC simulation, there were of two types: a) sand and b) biomass particles. The sand particles, as described in the previous section, were assumed to have a 100% SiO₂ composition with a PSD as described in Table 8-2. This was an exact match of the sand particles used in the experimental setup.

Concerning the 2.7 cm long and 0.7 cm of diameter wood pellets to be included in the simulations, it was observed that CFD-MPPIC simulations incorporate the following constraints: a) all computational particles involve clouds of particles and not individual particles, b) no particle...
can be larger than the cell size, with at least 10 particles per cell recommended (Benyahia et al., 2007).

Thus, and to be able to proceed with the CFD-MPPIC simulations, a particle with an assigned density equal to the biomass density and a 500 µm radius was considered. Using an agglomeration model, a 0.01 m diameter compact particle was created. This agglomerated group of particles was designated as a “Simulated Biomass Pellet.” Table 8-5 shows the input parameters of particles used in the CFD-MPPIC simulation. The size of this pellet was chosen to have the same volume as the experimental pellet without being bigger than each individual cell in the grid.

**Table 8-5. Input Parameters for Particles Used in a CFD-MPPIC Simulation.**

<table>
<thead>
<tr>
<th>Material</th>
<th>Density (kg/m³)</th>
<th>Sauter Mean Diameter (m)</th>
<th>Agglomeration Radius Cut Point (m)</th>
<th>Total Mass In Bed (kg)</th>
<th>Sphericity</th>
<th>Drag Model</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sand Particle</td>
<td>2650</td>
<td>520x10^-6</td>
<td>-</td>
<td>109</td>
<td>0.87</td>
<td>Parameterized Syamlal O’Brien (c1=0.547, d1=4.9972)</td>
</tr>
<tr>
<td>Biomass Particle</td>
<td>400</td>
<td>500x10^-6</td>
<td>0.005</td>
<td>0.648 (5 vol%) and, 1.29 (10 vol%)</td>
<td>0.8</td>
<td>Non-Spherical Ganser</td>
</tr>
</tbody>
</table>

### 8.5.2 Injection of Single Bubbles

Furthermore, once the input sand particles and simulated biomass pellet parameters were set for the simulation, the single bubble was injected into the bed. Based on the experimental data available for comparison (Torres Brauer et al., 2020), three single bubble volumes were selected for the analysis as follows: 336 cm³, 433 cm³, and 529 cm³. These bubble sizes will be designated as Bubble 01, Bubble 02, and Bubble 03, respectively, for each volume.
At the center of the bottom of the container used by CPFD Barracuda VR®, an 8 cm long bar was added in the axial direction. This injection post allows injecting single bubbles without a distributor effect. One should note that experimentally, single bubbles are created by filling a bubble injection cylinder of known volume with air at a certain pressure. This cylinder is connected to an injection point located inside the dense fluidized bed. By knowing the pressure at both ends of the injection system, and using the Bernoulli’s equation (61), the injection air velocity profile can be calculated.

\[
v_{\text{air}} = \sqrt{\frac{2(P_{\text{cylinder}} - P_{\text{ip}} - \rho_{\text{air}}g h_{\text{ip}})}{\rho_{\text{air}}}} \tag{61}
\]

where \(P_{\text{cylinder}}\) is the pressure inside the auxiliary injection cylinder, \(P_{\text{ip}}\) is the hydrostatic pressure at the injection port due to the weight of the sand and \(h_{\text{ip}}\) is the height of the injection port relative to the length of the bubble injection cylinder.

The calculated injection air velocity was employed to measure the air mass flow of the injected bubble through the nozzle at the injection point. Using this mass flow, the amount of air evacuated from the auxiliary injection cylinder in a small fraction of time was calculated. Then, the new corresponding pressure inside the auxiliary injection cylinder was established. With this new pressure, a new velocity and mass flow were calculated. The process was repeated until the auxiliary injection cylinder was empty. Additionally, the integral of the mass flow rate of the successive injected bubbles was calculated to determine the total injected mass of the bubble per injected volume. One should note that this total mass of injected bubbles was in close approximation (~99%) with the nominal mass of the injected bubbles during the experiments. Furthermore, the obtained mass flow profile was considered as the Boundary Condition as required by CPFD Barracuda VR®. One example of these mass flow rate profiles is given in Figure 8-5.
Figure 8-5. Calculated Air Mass Flow for Consecutive Injected Bubbles. Note: Mass balance for consecutive bubbles (∫ Ms dt) > 99% of the nominal mass of consecutive bubbles injected.

8.6 Numerical Data Treatment

Numerical data and experimental data can be mutually validated when the experiments are repeated through a simulator, and the results are similar. Not only can the experimental results be verified, but the input parameters of the numerical simulation can be recorded as those which can be used to scale or improve the process in a posterior step. All this implies that a comparison of the numerical and experimental results should be made. This can sometimes be a difficult task.

While the CREC Optiprobe system has a control volume that measures the bubble while passes through it, the same cannot be said for the CPFD Barracuda VR® software, which contains Transient Points, which act like sensors inside the simulated cold model.
CREC Optiprobe system can measure the particle volume fraction of the control volume via the contained particles reflected light and. Due to the size of this control volume, these measurements can be considered made in a singular point inside the bed. Bubble detection occurs when a bubble crosses the measurement point and impedes the reflection. *Transient Points* do not deliver data from singular points in the same way the CREC Optiprobe system does; they average the selected magnitude from the volume of the cell that contains them. Therefore, the particle volume fraction measured with a transient point will be affected by a bubble that enters its containing cell before the bubble crosses the actual sensor. Because of this, the signal produced by a transient point cannot be interpreted or treated in the same way as the one from the CREC Optiprobe system.

Due to this, it was opted to analyze the images produced by the simulator, which track bubbles from bubble injection point to the bubble reaching the bed surface.

This chapter explains the details of the treatment of the images generated by the simulator and how they were converted into bubble size, bubble shape, and bubble velocity.

### 8.6.1 Determination of Single Bubble Axial Chord and Rise Velocity from CFD-MPPIC Simulations

The objective of CFD-MPPIC single bubble simulations, used in this study, is the establishment of a Bubble Axial Chord (BAC) and the Bubble Rise Velocity (BRV) relationship within the bed free or loaded with biomass pellets.

In order to calculate both the BAC and the BRV, a series of images taken at every 0.1s was prepared using the CPFD Barracuda VR® simulation software. To acquire these images, the following steps were followed, as described in Figure 8-6: a) The 3D reactor model was sectioned
longitudinally, b) The resulting half-reactor section was reoriented to provide 2D like images. It is important to stress that these pictures do not correspond to a 2D bed but a 2D view image of a 3D bed. Thus, these images can be used to show the true dynamics of wall undisturbed bubbles, which would be difficult to illustrate in a 2D bed unit where bubbles are strongly affected by the walls.

Figure 8-6. Image Sequence Showing how a 2D Image of the Simulated Fluidized Sand Bed can be Obtained from a 3D Model. The cylinder is cut in half and reoriented to look like a 2D image.

Figure 8-7. Image Sequence of the CFD Simulation of a Single Bubble Rising in the Fluidized Sand Bed.
Figure 8-7 shows a sequence of images obtained with CPFD Barracuda VR® after the simulation was done. Once this sequence of images was obtained, each image was analyzed using a developed MATLAB code. This was done to extract the blue color region, which was the selected scale chosen to represent the volume devoid of particles. Once extracted from the frame, the centroid of the figure was identified, and two measurements were obtained: the horizontal diameter of the bubble and the vertical diameter of the bubble. On this basis, these measurements, both crossing the identified centroid, were calculated. This complete sequence of image data treatment is described in Figure 8-8.

![Figure 8-8. Data Treatment for Single Bubbles at t=5.5 s: a) Original image, b) Cropped image showing the dense phase sand bed only, c) Negative of the bubble image highlighted in “white,” d) Negative of the bubble image with the bubble centroid identified, e) Negative of the bubble image with horizontal axial bubble coordinates identified, f) Negative of the bubble image with vertical coordinates shown.](image-url)
The described method was applied to all CFD-MPPIC bubble simulations. Results obtained are compared in the upcoming sections of this study. Results are also compared with an alternate approach designates as the Hybrid Experimental-Spherical Cap (HESC) Method, as proposed by us in a recent study (Torres Brauer et al., 2020).

### 8.7 Conclusions

a) The drag model, the sand particles, and biomass pellet properties have to be carefully chosen.

b) Experimental and numerical bubble data must be obtained at the same bed location, so data can be compared effectively.

c) CFD-MPPIC simulations must be run for 20 seconds, injecting a bubble every 2 seconds following a 5-second lag time. As a result, eight (8) injected bubbles per run need to be studied.
Chapter 9: **Numerical Results and Discussion**

CPFD Barracuda VR© was used to carry out CFD-MPPIC simulations, as described in Chapter 8. The obtained series of data were processed following a methodology developed to be able to determine both the BACs and BRVs for single bubbles.

This chapter reports a summary of the findings of the numerical simulation of a sand fluidized bed and a comparison of these with experimental results.

**9.1 Single Bubble in Sand Fluidized Bed Without Biomass Pellets**

As a first step, and to establish the validity of the CFD-MPPIC simulation, a comparison with the Hybrid Experiment-Spherical Cap (HESC) Model data was developed with single bubbles injected in a bed without biomass. Figure 9-1(a), (b), and (c) show the changes of Bubble Rise Velocity (BRV) with Bubble Axial Chord (BAC). Findings from both the HESC Model and the CFD-MPPIC simulation are compared with Wallis (Wallis, 1969) and Rowe and Patridge's correlations (Rowe and Partridge, 1965).
Figure 9-1. Correlation Between BRV and BAC for Bubbles from the CFD-MPPIC Simulation and the HESC Model. Notes: a) Bubble 01: 336 cm³, b) Bubble 02: 433 cm³, c) Bubble 03: 529 cm³.

Figure 9-1a), 9-1b) and 9-1c) report that both the CFD-MPPIC simulations and the HESC Model predict close bubble sizes. However, the BRV data somewhat differs between sets of data, with this being particularly true for Bubble 03.

Given this discrepancy, the bubble Frontal Radius (FR) and the bubble BAC predicted by the HESC model and the CFD-PC simulation were compared, as shown in Figure 9-2.
Figure 9-2. Correlation Between the BAC and the FR of the HESC Model Bubbles and the CFD PIC Bubbles. For reference, the form factor BAC/FR=1.6, and 1 lines are also plotted.

Figure 9-2 shows that essentially all bubbles considered by both the HRSC Model and the CFD-MPPIC simulations are bracketed in between the BAC/FR of 1 and 1.6. However, the CFD-MPPIC simulated bubbles suggest a larger frontal radius. One should note that the BAC/FR=1.6, is an anticipated ratio for spherical cap-shaped bubbles as found in the HESC, with some variation of this ratio being due to the intrinsic randomness of bubbles.

Regarding the observed differences observed from CFD-MPPIC simulations and the data from a Hybrid Experimental-Spherical Cap (HESC) method, the following can be stated:

a) CREC-Optiprobe measurements, as per the HESC, yield bubble data at fixed positions, while CFD-MPPIC bubbles are followed along the bed and evaluated every 0.1s.

b) The Bubble Rise Velocity (BRV) obtained with the HESC is calculated using the time needed for the front of the bubble to cross two probes located at two set positions. The CFD-MPPIC, on the other hand, measures BRV more rigorously by locating the bubble centroid and measuring its changing position over time. This may create differences between BRVs as a result of bubble deformation.
c) Bubbles injected can have intrinsic randomness, drifting from the center of the fluidized bed, where the control volume of the CREC-Optiprobe system is located, causing the system to measure smaller bubbles or not detect them at all. The CFD-MPPIC, in conjunction with the MATLAB software, tracks bubbles, regardless of its radial position.

d) The bubble frontal radius, in the HESC, is based on video camera images that measure the bubble’s “footprint” at the bed surface during its ascension and rupture. Due to a possible misleading effect of the bubble roof over the walls of the footprint, as reported by Levenspiel (Kunii and Levenspiel, 1991), an extrapolation was made to compensate for the size change in the image. In the case of the CFD-MPPIC simulation, the frontal radius is measured directly without aberrations due to the bubble roof collapse.

Regarding the BRV velocity as reported in Figure 9-1a), 9-1b) and 9-1c) and the insights provided by the CFD-MPPIC simulations, it was noticed that the bubble shape changed while bubbles moved through the bed. For instance, it was observed that it was easy for bubbles with a larger form factor to transit through the bed due to their smaller frontal area, and having as a result, a higher BRV for the same BAC. As well, it was also observed that it was harder for small form factor bubbles to evolve in the bed due to their larger area that opposes to their movement, leading to a smaller BRV. As one can see in Figure 9-2, HESC Model bubbles tended to stay closer to the 1.6 form factor line given their assigned spherical cap geometry while CFD-MPPIC bubbles tended to drift to a BAC/FR of 1 given their flatter bubble geometry.

Thus, one can conclude that the HESC Model and CFD-MPPIC simulations are both valuable and complement each other. The HESC Model based on a set of two CREC Optiprobes readings, provides a first-order bubble dynamic assessment while the CFD-MPPIC gives a detailed
simulation of bubble dynamics. Each of them certainly involves a different effort in terms of experimentation and computer simulation.

**9.2 Single Bubbles in Sand Fluidized Bed Loaded with Biomass Pellets**

Given the significant value of predicted bubble dynamics in sand beds loaded with biomass pellets particles, both the HESC Model and CFD-MPPIC simulations were considered under these conditions.

Figure 9-3a), 9-3b), and 9-3c) provides this comparison. Thus, one can see that once biomass pellets are added to the sand fluidized bed, the behavior of the bubbles changed significantly, shifting to smaller and slower bubbles according to the HESC model. Furthermore, one can also observe in Figure 9-3a), 9-3b) and 9-3c) that most of the HESC Model and CFD-MPPIC simulated bubbles are not bracketed by the correlation of Wallis (Wallis, 1969) and Rowe and Partridge (Rowe and Partridge, 1965), with these correlations consistently overpredicting the BVR.
Figure 9-3. Comparison between BRV and BAC for Bubbles in Sand Fluidized Beds Loaded with Biomass Pellets using the HESC Model and CFD-MPPIC Simulations. Notes: a) Bubble 01 (336 cm³) with 5 vol% and 10 vol% of Biomass Pellets, b) Bubble 02 (433 cm³) with 5 vol% and 10 vol% of Biomass Pellets.

One can also see, as shown in Figure 9-3a), 9-3b) and 9-3c) that both the HESC Model and the CFD-MPPIC simulations yielded BACs within the same ranges. Furthermore, and regarding the observed BRV values for both the HESC Model and the CFD-MPPIC simulations, one can notice that they are in a close range for Bubble 01, displaying moderate differences for Bubble 02 and Bubble 03.
It can also be noticed, as in the case of the fluidized bed without biomass, as discussed in Section 9.1, that the CFD-MPPIC simulation tends to give slower bubbles, than the ones calculated with the HESC Model. Reasons for this difference between the CFD-MPPIC and the HESC predictions can be assigned to changes from the spherical cap shape hypothesized by the HESC.

Thus, one can conclude that for sand fluidized beds with 5 vol% and 10 vol% of biomass loadings, the HESC Model and CFD-MPPIC simulations complement each other. The HESC Model is a valuable and practical approximation for a bubble dynamics assessment, in a continuous biomass gasifier. The CFD-MPPIC simulation, which is quite intense in computations, on the other hand, provides a detailed and accurate description of bubble dynamics. These combined approaches are of importance if one considers the joint application of the CREC Optiprobes with CFI-MPPIC simulations for the design and operation of a continuous sand-biomass fluidized bed gasifier.

9.3 Conclusions

a) The adopted CFI-MPPIC methodology to track bubbles was found to be effective and reliable.

b) The input parameters selected, and bubble injection mode considered for the CFI-MPPIC simulation were adequate to reproduce experimentally observed BRVs and BACs.

c) The numerically calculated BACs were in very good agreement with the HESC model calculations.

d) The numerically calculated BRVs consistently under-predicted the BRV from the HESC model. This was be attributed to bubble deformation.
Chapter 10: **Sand Bed Dense Phase Bubbling Fluidization**

While the information reported in Chapter 7 and 9 for single bubble injections and their posterior numerical simulation, is relevant for bubble flow phenomenological analysis, the operation of a sand fluidized bed gasifier and its scaling up under dense phase fluidization conditions is still a challenging issue.

In fact, when multiple bubbles are present in the reactor, the interaction between bubbles can change the overall fluidized bed behavior. Bubble splitting, bubble coalescence, and bubble deformation are common events that may take place inside the column.

Given all the above, it is of great interest to establish suitable numerical approaches to simulate sand beds under dense phase fluidization conditions in beds with and without loaded biomass.

### 10.1 Experimental Results and Discussion

Regarding studies with the sand fluidized bed operating under dense phase fluidization conditions, the various components of the experimental setup described in Chapter 4, were used. The airflow, however, was well above minimum fluidization. Prior to the experiments with and without biomass loaded, the gasifier cold model unit was first fluidized for a 5-minute period. This was done to reach a stabilized operating condition. Then, measurements were performed by fluidizing the gasifier cold model unit for another 5 seconds and recording the data at 1000 Hz.

In the case of runs which included biomass pellets, the wood pellets were added in the bed first. Following this, the bed was fluidized at 90 SCFM, which is the maximum achievable airflow in the experimental system. This was done for 2 minutes to achieve a homogeneous solid mixing. Then, the air volumetric flow was reduced to the one selected for the experiment. After 2 minutes
of stabilization, data collection from the experimental setup was initiated. In all cases, the homogeneous mixing of sand and pellets was visually confirmed.

The air volumetric flows selected for the runs were 60, 70, and 80 SCFM. These volumetric flows corresponded to 0.0334, 0.0391 and 0.0447 kg/s gas mass flows and to 0.19, 0.22 and 0.25 m/s superficial gas velocities. One should note that in the present Chapter, the airflow used in various experiments was designated with SCFM units for reporting results.

Figure 10-1 describes the effect of increasing the air volumetric flow on both the BAC and the BRV.

![Graphs](image.png)

**Figure 10-1. a) Averaged BAC Measurements and b) Averaged BRV Measurements for Bubbles in a Sand Fluidized Bed under the Dense Phase Fluidization Conditions at Different Radial Positions and Given Volumetric Flows.**

Based on Figure 10-1 data, one can see that both the averaged BAC and the averaged BRV values increase with the radial position, with BACs and BRV being close to zero at the near-wall region and augmenting progressively as one approaches the center of the unit.

One can observe in Figure 10-1, that averaged BACs and averaged BRVs augment away from the walls and for higher volumetric flows. This behavior is consistent with the description of
Levenspiel (Kunii and Levenspiel, 1991), which assigns to bubbles under dense phase fluidization, the excess flow with respect to the one required minimum fluidization. Thus, injecting higher volumetric flows gives bigger bubbles with higher buoyancy and therefore, higher velocity.

Figure 10-2 describes the effect of adding biomass pellets to the bubble flow both in terms of the BAC and the BRV.

Figure 10-2 reports the biomass pellet addition effect. It decreases both the BACs and the BRVs. For instance, one can see that adding 25 vol% of biomass to 70 and 80 SCFM fluidization air flows, reduced both BACs and BRVs. For the bed loaded with biomass pellets, this finding was more apparent at the bed center than at the bed near-wall region.
Figure 10-3 reports the correlation between experimentally measured BRVs and BACs for individual bubbles in a dense phase fluidized bed at a) 60 SCFM with 0 vol% biomass, b) 70 SCFM with 0 vol% biomass, and c) 80 SCFM with 0 vol% biomass. Full and dotted lines reported in these figures, corresponding to various correlations reported in the literature, as already discussed in Section 2.1.

One can thus see in Figure 10-3 that for all the measured bubbles, there is a bubble fraction falling in the underpredicted band. This BAC underpredicted band fraction is assigned to bubbles...
moving slower than the ones expected for their corresponding BACs. This phenomenon is assigned to bubble deformation, with bubbles geometry becoming flatter. On the other hand, some other bubbles fall in the BAC overpredicted fraction band category, with these bubbles moving faster than anticipated given their BACs. This behavior was assigned to the following: a) Smaller bubbles being pulled up by bigger bubbles moving in front of them, forming a bubble train, b) Bubbles contacting the CREC Optiprobess off-center, and being detected as having a smaller BAC.

Thus, one can conclude that available BAC versus BRV correlations are unable to represent bubble dynamics in a sand fluidized bed. This shows the need for a new BAC correlation model versus a BRV correlation model, which included a probabilistic component, which will account for the randomness of the bubble flow.

10.2 Numerical Approach to the Bubbling Fluidization Regime

Up to this point, in the present Ph.D. dissertation, the dynamic behavior of numerically calculated single bubbles, injected at the bottom of a bed with a grid having a geometry as shown in Figure 10-4 a) was considered as follows: a) single bubbles were injected via a central nozzle, b) a secondary airflow was fed using a perforated plate, which kept the sand at near-minimum fluidization.

Thus, the next step in the present study was to consider the numerical calculation of a swarm of bubbles now injected via the perforated grid plate, with the bed being under the dense phase regime. In this case, the gas flow was well above minimum fluidization. Numerical simulation of these conditions showed an almost total bubble absence in the near-wall region. This was partially assigned to the air distributor configuration, given that the exact distributor arrangement could not be accurately considered, as a result of the following constraints: a) The selected numerical cell could not be smaller than the larger bigger particle, b) The geometry considered by the CFD-
MPPIC software was the result of the intersection of the selected grid and the 3D model, which was provided by the user (CPFD Software LLC., 2019). In this regard, one should note that given the 2mm diameter grid, the air inlets did not provide enough grid specifics while considering 1 cm³ biomass pellets.

Thus, the following steps were chosen as shown in Figure 10-4b): a) To use an approximation to the nozzles as described in Section 4.2, by constructing cylinders in the distributor plane, b) To use their top surfaces as air inlets. This approach was found to be adequate for simulating experimental results and bubble locations.

Figure 10-4. Images Generated by CPFD Barracuda VR® Showing the Geometry Used to Simulate the Fluidized Bed, where the Red Zone Represents the Air Inlet and the Yellow Zone Represents the Pressure Outlet. a) Using the bottom surface as an air inlet and b) Using only cylinders as air inlets to better represent the distributor.
Using this strategy, all experimental runs were simulated using CFD-MPPIC Barracuda®. The air input was chosen using volumetric flows, consistent with the nominal mass flows selected for the experimental runs. The rest of the input parameters were selected, as reported in Table 10-1.

Regarding CFD-MPPIC Barracuda® simulations, the *Transient Points* software feature was used. This allowed virtual sensors to be placed inside a given cell, replicating experimental measurement points. This was done starting from the fluidized bed centerline and scanning the bed in the radial direction every 3 cm until the unit wall was reached.

Furthermore, 8 *Transient Points* were used to measure cell particle volume fractions along the radius of the main column and near the surface at two different heights: 38cm and 40 cm bed above the distributor. The particle volume fraction data produced by the *Transient Points* was processed with the same MATLAB program as for the experimental results. Some minor modifications were introduced, to account for the different inter-sensor distances and the different noise levels of the resulting signals.
### Table 10-1. Input Parameters Used to Simulate the Bubbling Regime on the Sand Fluidized Bed Biomass Gasifier.

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</table>

10.3 Numerical Results and Discussion

The numerical simulation of the dense phase sand fluidized bed cold model unit, operated with continuous air feeding via a perforated plate, was developed, as already described in Section 8.4.
A comparison of experimentally obtained results with a CPFD-MPPIC Barracuda © simulation was of critical value for model validation. This approach is of major importance for evaluating simulation conditions when biomass is added to the sand fluidized bed. With this end in mind, BACs and BRVs for bubbles generated during fluidization were measured experimentally with the HESC model and simulated via CPFD Barracuda VR®. The biomass effect was also included in this analysis.

Figure 10-5 a) and b) report simulation results in the case of a sand bed without biomass pellets loaded.

![Figure 10-5](image)

*Figure 10-5. a) Averaged BAC and b) Averaged BRV Measurements of Simulated Bubbles using CFD-MPPIC at Different Radial Positions and Given Volumetric Flows.*

Figure 10-5 displays both averaged BACs and averaged BRVs, showing a higher bubble density at the central radial positions and close to no bubbles at the near-wall region. It can also be noticed that when the gas volumetric flow was increased from 60 SCFM to 80 SCFM, this led to larger and faster bubbles.
Figure 10-6 reports a comparison between experimentally and numerically obtained BACs for: a) 60 SCFM with 0 vol% biomass, b) 70 SCFM with 0 vol% biomass and c) 70 SCFM with 25 vol% of biomass, d) 80 SCFM with 0 vol% of biomass and e) 80 SCFM with 25 vol% of biomass.

Figure 10-6. Comparison between Experimental and Numerical BACs at Different Radial Positions from the Wall (r/R=1) to the Bed Center (r/R=0) for: a) 60 SCFM 0 vol% biomass, b) 70 SCFM 0 vol% biomass, and c) 80 SCFM 0 vol% biomass. The solid black lines represent experimental values, and the solid red lines represent numerical values.
Figure 10-6a), b), and c) show that the experimentally measured BACs and the numerically obtained BACs are close in all cases, displaying the same trend along with the various radial positions. The minor observed differences between BACs can be attributed to the intrinsic randomness of the bubble flow, already discussed in Chapter 6.

Figure 10-7 a) and b) report the experimentally measured BACs and the numerically calculated BACs at different radial positions, in a sand fluidized bed using a 70 SCFM gas flow with a 25 vol% loading of biomass added.

**Figure 10-7. Comparison between Experimental and Numerical BACs at Different Radial Positions from the Wall (r/R=1) to the Bed Center (r/R=0) for a) 70 SCFM 25 vol% biomass and b) 80 SCFM 25 vol% biomass. Notes: a) The solid black lines represent experimental values, b) The solid red lines represent numerical values.**

Figure 10-7a) and b) display show again the small differences between experimental and numerical BACs, with this being a positive indicator of the validation of the PIC-CFD Barracuda simulations while biomass was loaded in the bed.
Figure 10-8a), b) and c) report a further comparison between experimentally and numerically obtained BRVs, with no biomass added to the bed and at the following conditions: a) 60 SCFM, b) 70 SCFM, and c) 80 SCFM.

Figure 10-8. Comparison between Experimental and Numerical BRVs at Different Radial Positions from the Wall (r/R=1) to the Bed Center (r/R=0) for: a) 60 SCFM 0 vol% biomass, b) 70 SCFM 0 vol% biomass, and c) 80 SCFM 0 vol% biomass. Notes: a) The solid black lines represent experimental values, b) The solid red lines represent numerical values.
Regarding Figure 10-8a) b), and c), one can observe the excellent similarity between experimentally measured and the numerically obtained BRVs at 60 SCFs. This is consistent with the conclusions reported in Chapter 9, where it was found that the CFD-MPPIC method is adequate to replicate experimental BRVs for the smaller bubbles studied.

Furthermore, Figure 10-8b) and d) show BRVs for 70 and 80 SCFM in a bed with 25 vol% biomass. Here, the agreement is less apparent, with BRVs being similar near the center of the bed and less comparable close to the unit walls, with CPFD Barracuda VR® overpredicting BRVs.

Finally, Figure 10-9a) and b) describe average BRVs both numerically calculated and experimentally measured for 70 SFM and 80 SFM air flows and a bed loaded with 25vol% of biomass.

![Figure 10-9. Comparison between Experimental and Numerical BRVs at Different Radial Positions from the Wall (r/R=1) to the Bed Center (r/R=0) for a) 70 SCFM 25 vol% biomass and b) 80 SCFM 25 vol% biomass. Notes: a) The solid black lines represent experimental values, b) The solid red lines represent numerical values.]

As illustrated in Figure 10-8a) and b), the numerical BRVs and the experimental BRVs display the following features: a) BRV profiles for numerically calculated and experimentally
measured bubbles display a parabolic shape, being quite flat in the central section of the bed, b) The numerically calculated BRVs consistently overpredict the experimentally observed BRVs.

Thus, and based on the results obtained, one can conclude that: a) The CFD-MPPIC simulation is able to predict both BACs and BRVs adequately in sand fluidized beds free of biomass and b) The CFD-MPPIC model for 25 vol% pellets in sand fluidized beds can simulate BACs well yet, is less reliable to calculate BRVs.

As a result, it can be postulated that in the sand-biomass pellet media, the CFD-MPPIC simulations, while computing BACs very close to experimentally measured ones, call for a modification of the drag coefficient for BRV evaluations. This modified drag coefficient should be carefully reassessed, making the computed BRV values more consistent with the lower experimentally observed BRVs.

10.4 Conclusions

a) BAC and BRV available correlations, while applied to dense phase sand fluidized beds, show that they can describe a limited number of bubbles only. This finding calls for new BAC-BRV correlations, with these correlations including probabilistic parameters and capturing the randomness of the bubble flow.

b) CFD-MPPIC Barracuda numerical calculations in sand fluidized beds without added biomass, at various radial positions and air gas flows, show good agreement with experimental results, for both BACs and BRVs. This result is a relevant one, given the prospects of having a reliable simulation software for scaling up biomass sand fluidized beds, of a size compatible with the ones expected in biomass gasification plants.
c) CFD-MPPIC Barracuda numerical calculations in sand fluidized beds with added biomass pellets show good BACs predictions. However, obtained BRVs consistently overpredict experimental results. This observed discrepancy with numerically calculated bubbles being faster than experimentally observed ones, calls for modifications of the drag coefficient correlation included in CFD-MPPIC Barracuda model. This change could favorably account for the extra drag introduced by biomass pellets in the bubble flow.
Chapter 11: Conclusions and Recommendations

11.1 Conclusions

11.1.1 Experimental Data

A combined CREC-Optiprobos and video camera methodology were employed to study bubbles in sand fluidized beds. Based on the data obtained, the following can be concluded:

a) It is proven that this methodology can be applied successfully to examine peaks recorded by two axially aligned CREC Optiprobos. Effective data treatment involves setting a signal baseline, which allows for bubble sizing and bubble velocity calculations. The proposed method is validated via an injected gas volume balance.

b) It is shown that the proposed approach can be used for establishing tridimensional bubble geometries and their inner bubble interfaces. The resulting bubbles with “cap” shapes and a wavy inner interface are in agreement with MRI measurements developed by others (Boyce et al., 2019).

c) It is demonstrated that the proposed methodology can be employed in sand fluidized beds using analog biomass pellets in the 5 vol%-10 vol% range. This shows that calculated BACs are consistently reduced with increased biomass loadings.

d) It is proven that all BAC and BRV data recorded, with and without biomass loaded in sand fluidized beds, can be correlated with a single relationship where the BRV changes proportionally to the square root of the BAC.

e) It is shown that even if the biomass pellets reduced the BAC, the normalized BAC distribution functions observed in the bed free of biomass, remains as well unchanged in beds with analog biomass pellets.

CFD-MPPIC numerical simulations were successfully developed to study single bubbles in a sand fluidized bed with and without biomass pellets. This was done to assess the effect of the biomass pellets on bubble dynamics. The CFD-MPPIC simulation used the Parameterized Syamlal O’Brien Drag Model, given its ability to reproduce the experimentally measured minimum fluidization velocity. This allowed single bubble simulations to be consistent with the experimentally measured data. Furthermore, the CFD-MPPIC simulations considered pellets formed using a particle agglomeration model and a MATLAB program for the processing of CFD-MPPIC bubble images. On the basis, the following can be concluded:

a) The CFD-MPPIC simulations can be favorably compared with a HESC (Hybrid Experimental-Spherical Cap Bubble) Model, which includes experimental data obtained in a 0.4 m diameter sand fluidized bed using the CREC Optiprobes. The BACs obtained in the CFD-MPPIC simulations for the 336 cm$^3$-529 cm$^3$ bubbles injected, show good agreement with the BACs from the HESC Model.

b) The CFD-MPPIC simulations display BRVs consistently lower than those for the HESC bubbles, for sand fluidized bed simulations both with and without biomass pellets loaded. This discrepancy is assigned to the restricted applicability of the spherical cap-shaped bubbles, as assumed by the HESC Model.
11.1.3 Bubbles in a Bubbling Sand Fluidized Bed

The sand fluidized bed in the dense phase bubbling regime was further studied using both CREC-Optiprob® and CFD-MPPIC numerical simulations with and without biomass pellets. Based on this study, the following can be concluded:

a) Bubble sizes and bubble velocities encompass wide distributions.

b) Bubbles could grow due to coalescence and be reduced in size due to bubble split.

c) Bubble BAC and bubble BRV follow a correlation like the one for individual bubbles, with some bubbles falling outside the anticipated error band. This is attributed to the bubble position randomness at contact points with CREC Optiprob®.

d) BACs can be predicted with accuracy using CFD-MPPIC simulations, in the case of bubbles evolving in a sand fluidized bed operating in the bubbling dense phase regime, with and without added biomass.

e) BRVs can also be obtained with accuracy using CFD-MPPIC simulations for the smallest bubbles in the bed. This simulation is less reliable, however, for the largest bubbles studies.

f) BRVs predictions using CFD-MPPIC simulations become less trustable when biomass pellets are added to the sand fluidized bed.
11.2 Recommendations

a) The experimental information obtained with the CREC-Optiprobes should be extended to different types and shapes of biomass.

b) The bubble data treatment should be modified to implement computer vision to track and measure bubbles. This could be done either from experimental footage generated with non-intrusive imaging or generated with a CFD software.

c) The HESC model used to treat the experimental data should be modified to remove the constraint imposed on the combined bubble-wake of being of spherical.

d) The particle-drag equations available in CFD-MPPIC should be modified to account in bubbling sand fluidized beds with added biomass particles, for the slower experimentally BVR observed.

e) Improvements should be included in CFD-MPPIC simulations for properly accounting biomass shape and hardness.
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Single-Bubble Dynamics in a Dense Phase Fluidized Sand Bed Biomass Gasification Environment

Author: Nicolas Torres Brauer, Benito Serrano Rosales, Hugo de Lasa
Publication: Industrial & Engineering Chemistry Research
Publisher: American Chemical Society
Date: Apr 1, 2020

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Curriculum Vitae

Name

Nicolas Torres Brauer

Post-Secondary Education and Degrees

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<td>1st place Award Oral Presentation</td>
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<td>4 times elected Teacher Assistant of the Year</td>
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Refereed Publications

