Dancing with Bubbles: Deterministic versus Probabilistic Bubble Models in Dense Phase Sand Fluidized Beds for Biomass Gasification

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Abstract: This study addresses the need to model bubble flow in a fluidized bed using a probabilistic approach, which includes intrinsic bubble flow randomness. It is shown that the proposed probabilistic predictive model (PPM) overcomes the limitations of deterministic correlations, commonly used to describe bubble dynamics in high-density (above 2000 kg/m$^3$) sand-beds of Type B particles of the Geldart classification. It is proven that a PPM can describe the relationship between bubble axial chord and bubble rise velocity using minimum and maximum behavioral bands. This probabilistic model, which applies to a wide range of operating conditions, as shown in the present study, can be considered applicable to single bubbles injected at incipient fluidization, as well as to bubbly beds with and without loaded biomass pellets.

Keywords: bubbling fluidized bed; probabilistic predictive model; gasification; sand fluidization; bubble rise velocity; CREC optical fiber probe

1. Introduction

The gasification of biomass in a fluidized bed is an efficient and fast way to transform agricultural waste and other biomass sources into synthesis gas, also known as syngas [1–3]. While the collection of tar formed and the particles are potential issues, as has been well documented by others [4–7], adequate cyclones and filters in gasifiers can help in providing clean green energy, since synthesis gas can be used to produce liquid fuels, chemicals of high value, and other forms of energy vectors. Given the importance of green alternative energy and the means to produce these valuable chemicals, the process of the gasification of biomass in a fluidized bed must be studied further under specific operating conditions.

The use of coarse sand particles of the Geldart Type B [8] in dense phase fluidized beds is adequate for gasifying biomass, given that it simplifies the separation of gases from ash and char. Despite this advantage, most of the hydrodynamic studies found in the literature are conducted with Geldart Type A and low-density (under 2000 kg/m$^3$) Type B powders, as discussed by Torres Brauer in 2020 [9].

One way to study fluidization is to analyze the gas motion through the bed as bubbles, and its effects on the fluidized particles. Bubble motion in beds of coarse sand particles is an increasingly important subject, given its relevance for bed mass and heat transfer.

Regarding single bubble motion in a fluidized bed, it has been reported [10–12] that a fluidized bed can be represented using a bubbling gas in a low viscosity liquid. These authors proposed a model to correlate the air bubble sizes with their rise velocity or BRV. They used the bubble nose-radius to report the bubble size, given that the bubble was considered to have a spherical cap shape and not a spherical shape. This model is expressed...
in Equation (1), where the bubble’s nose radius \( R_n \) is the parameter that characterizes the bubble size.

\[
BRV = \frac{2}{3} \sqrt[3]{gR_n} 
\]  
(1)

Later, this model was adapted by Davidson and Harrison [13] using experimental data from a 0.0152 m diameter bed with solid particles of a size distribution between 150 µm and 400 µm. These authors derived a revised model represented by Equation (2), which was limited to bubble-to-bed diameter ratios inferior to 0.125. This allowed bubbles to be measured in a way that was virtually unaffected by the unit walls. The BRV was correlated with the \( d_{b_{eq}} \), which represents the diameter of an equivalent spherical bubble with the same volume as the air volume contained in the spherical-cap shaped bubbles observed.

\[
BRV = 0.711 \sqrt{gd_{b_{eq}}} 
\]  
(2)

In 1969, Wallis [14] expanded the model shown in Equation (2), by including the effect of the reactor walls on the bubble, for the 0.125 to 0.6 \( d_{b_{eq}} / D \) ratio, as shown in Equation (3) with \( D \) being the reactor diameter:

\[
BRV = \left( 0.711 \sqrt{gd_{b_{eq}}} \right) 1.2 \exp \left( -1.49 \frac{d_{b_{eq}}}{D_{bed}} \right) 
\]  
(3)

Furthermore, Rowe [15,16] developed two models: one for particles of the Geldart Type B, shown in Equation (4), and another for Geldart Type A and B particles, as reported in Equation (5). These models take into consideration the particle diameter \( d_p \) instead of the vessel diameter:

\[
BRV = 1.02 \sqrt{gd_{b_{eq}}} 
\]  
(4)

\[
BRV = \left( 1.38 - 0.00182d_p \right) \sqrt{\frac{gd_{b_{eq}}}{2}} 
\]  
(5)

Allahwala and Potter [17] proposed a modified BRV model, which included the ratio of a bubble diameter over a reactor diameter, with this ratio being included in the argument of a hyperbolic tangent function, as shown in Equation (6):

\[
BRV = 0.35 \sqrt{gD_{bed}} \times \left( \tanh \left[ 3.6 \left( \frac{d_{b_{eq}}}{D_{bed}} \right)^{0.97} \right] \right)^{0.555} 
\]  
(6)

In 2011, Karimipour and Pugsley [18] compared various sets of experimental data with the available BRV models as described in Equations (1)–(6). They concluded that Wallis’s model, represented by Equation (3), was the closest to their experimental results. Most of these models, however, were derived from experimental results obtained from Type A and low-size (below 150 µm) Type B particles.

While many studies have been developed to determine bubble size and bubble velocity using deterministic-based correlations as described above, the present study aims to establish a different approach, with correlations incorporating a probabilistic factor that accounts for fluid motion randomness. This approach is considered in the present study, first, for single bubbles injected in a sand bed at incipient fluidization. It is extended later to bubbly sand fluidized beds, with several bubbles evolving simultaneously. The developed PPM is of particular importance for high-density beds (2000 kg m\(^{-3}\) – 3000 kg m\(^{-3}\)) of Type B particles of the Geldart classification, and for the scale-up of sand fluidized beds used in the production of syngas from agricultural waste. This represents a new way of modelling flow phenomena in fluidized bed reactors, where the intrinsic randomness of the bubble flow is included in the bubble phase description. The use of this approach can have a considerable impact on the nature of two-phase fluidized bed gasifier unit models.
accounting for both heterogenous and homogeneous reactions as follows: (a) chemical species balances in the dense phase; (b) chemical species balances in the gas phase based on the PPM; and (c) link between dense and bubble phases accounting for chemical species transport via bubble interfaces, as determined by the PPM.

2. Experimental Setup and Data Treatment

Single bubbles can be formed as in the present study, via the injection of a controlled amount of air through a nozzle located at the center of a cylindrical fluidized bed (42 cm of diameter) at a set height (0.1 m) above its distributor plate. During the runs, the bed was operated at room temperature and near to atmospheric pressure while kept under incipient fluidization conditions (IFC). The SiO₂ sand particles showed a PSD in the 200 µm to 900 µm range with a 580 µm mean diameter. On the other hand, added cylindrical pellets with a 2.7 cm length and 0.7 cm diameter were employed. Pellet addition was defined using bed volumetric concentrations (e.g., 5 vol%).

The single formed bubble is measured in our study, using the CREC-Optiprobe system. The CREC-Optiprobos are engineered to transmit a laser beam via one optical fiber (emitting fiber) into the sand bed to a second adjacent fiber (receiving fiber) that captures the light reflected from sand particle surface, transmitting it to a light sensor. The CREC-Optiprobos are completed with an A/D card and a PC computer for data processing. This approach allows one to measure local variations of the bed’s particle volume fractions. When the particle volume fraction is low, the laser’s reflection from the bed particles is negligible. On the other hand, when the particle volume fraction is high, the laser light reflected from the particles is quite substantial and measurable. Thus, changes in the local particle volume fraction in a dense phase fluidized bed can be tracked with laser light reflected variations as recorded by the CREC-Optiprobos and their associated optoelectronic system. Additional information regarding CREC-Optiprobos can be found in Torres Brauer (2020) [9].

Regarding fluidization conditions, incipient fluidization (IFC) can be achieved by selecting an air flow leading to the onset of bubbling in the bed, with no bubbles being observed at the upper bed surface (Torres Brauer et al., 2020) [19]. By using IFC, one avoids having multiple bubbles rising in the bed, while being able to simultaneously track a single injected bubble. As shown in Figure 1, under these conditions, one can record the single bubble motion, via measurements of both the bubble axial chord (BAC) and bubble front radius (BFR) by using both the CREC-Optiprobos and a video camera. In this study, once the data are acquired from the CREC-Optiprobos system and the video camera, they are processed using a Hybrid Spherical-Cap-Experimental model (HSCE model), developed by Torres Brauer et al. [19].

The HSCE model involves a geometrical description of single bubbles. It was developed to interpret the data obtained by CREC Optiprobos and camera video images. Since the CREC Optiprobos give the bubble vertical length and the upper placed video camera gives the projected bubble horizontal diameter, a geometrical bubble shape and bubble volume can be determined. On this basis, bubble volumes can be established using two parameters: the piercing bubble distance or bubble axial chord (BAC) and the bubble frontal radius (FR) (Figure 2), as reported in Torres Brauer et al. [18].

Once the HSCE model is established and validated, the bubble rise velocity (BRV) can be calculated. This is the case given that two CREC-Optiprobos are simultaneously used, with these two probes being separated vertically by a known distance.

On this basis, plots relating the BRV and BAC can be developed and compared with those reported in the technical literature. This analysis involves a bubble equivalent diameter which is calculated using the diameter of a spherical bubble of equal volume to the one of the spherical cap bubble [19].

\[ \text{BAC} = (0.7791) \, d_{boi} \]  \hspace{1cm} (7)

Equation (7) can be used further to transform Equations (1)–(6) into BRV versus BAC correlations. This was carried out in a previous study by our research team, in order to be
able to comprehensively compare proposed literature correlations with our experimental data [19]. In the case of Equation (1), the bubble’s nose radius was assumed to be the same as the frontal radius according to the HSCE model [19]. In this manner, a relationship is established between $R_n$ and BAC.

![Figure 1](image1.png)

**Figure 1.** Fluidized bed unit operated at room temperature and near to atmospheric pressure by Torres Brauer (2020) [9]. Details provided show the position of the CREC-Optiprobe sensors.

![Figure 2](image2.png)

**Figure 2.** An axial cross-section of the HSCE model bubble. The white region represents air, and the black region represents the wake (a mix of air and sand) (Adapted from Torres Brauer et al. [19]).

### 3. Current Available Models and the Experimental Data Fitting

Figure 3 reports the BRVs and BACs of single injected bubbles of different sizes. Sizes 1 to 4 were $336 \times 10^{-6}$ m$^3$, $433 \times 10^{-6}$ m$^3$, $529 \times 10^{-6}$ m$^3$, $626 \times 10^{-6}$ m$^3$. Bubbles were measured as described in the previous section, and as shown in various reported technical literature correlations [19–23]. It is apparent from Figure 3 that there is no overall fair fit for bubbles, among the known proposed correlations. Smaller bubbles (0.05–0.07 m) show a good fit with Allahwala and Potter’s research (Equation (6)), and Wallis’s models (Equation (3)). However, as bubbles grow, they start differing significantly from these models, and approximate those predicted by Rowe and Partridge (Equation (4)), and Rowe and Yacono (Equation (5)).
Furthermore, and regarding the data reported in Figure 3, one can also notice an intrinsic randomness in the injected and detected bubbles. One can argue that bubble dynamics, characterized by bubble size and bubble velocity, are better represented by a range limited by minimum and maximum values. These values are assigned to the somewhat disordered bed medium where bubbles are formed first and evolve later until they reach the upper bed surface. It is our view that this intrinsic fluidized bed probabilistic behavior cannot be accounted for with deterministic models solely, such as those available in the technical literature. It requires models that incorporate the inherent fluidized bed randomness.

4. The Probabilistic Predictive Model (PPM)

Torres Brauer et al. [19] recently proposed the use of Equation (8) to predict the size of the injected single bubbles, regardless of the presence or absence of biomass where $\gamma$ is an empirically determined coefficient with a $0.86 \pm 0.00975$ value.

$$BRV = \gamma \sqrt{\frac{\Omega}{g}} BAC$$

(8)

Due to the randomness of the BRV bubble velocity and the wide variation of bubble sizes observed, during both experiments and simulations, adding a Probabilistic Coefficient ($\Omega$) to Equation (8) was proposed.

This $\Omega$ coefficient transforms the deterministic model described by Equation (8) into a PPM probabilistic predictive model (PMM) including a randomness term, as described in Equation (9). Additionally, the $\frac{\Omega}{g}$ particle volume fractions ratio included in the model is considered to describe the change in bubble drag as a result of bubbles moving in a lean bed at higher airflow.

$$BRV = \Omega \left(\frac{\epsilon_{IFC}}{\epsilon} \right)^n \sqrt{\frac{\Omega}{g}} BAC$$

(9)

with $\epsilon_{IFC}$ being the particle volume fraction at incipient fluidization [12] with a value of 0.47, with $\epsilon$ representing the average bed particle volume fraction during a run, and with $n$ denoting the adjusted empirical exponent with a value of 3.5. The coefficient ($\gamma$) from Equation (8) is used again but after further refining, its value lowered to 0.748.

One should note that the probability distribution coefficient ($\Omega$) in Equation (9) of the PPM involves the following:

(a) A relative signed error (RSE) that can be calculated for every experimental data condition, using the BRVs calculated with Equation (8). On this basis, one can define a standard deviation of the individual BRV data series of errors ($\sigma_{RSE}$);
(b) A probabilistic predictive band, delimited by one standard deviation of the relative signed error series \((+/−σ_{RSE})\). For instance, if \(σ_{RSE} = 0.26\), the values considered for \(Ω\) fall in between \(0.74 < Ω < 1.26\) range;

(c) A BRV normal error distribution, given the anticipated flow randomness, as determined by Equation (10) as follows:

\[
Ω = \frac{1}{\sqrt{2π}} \exp \left\{ \frac{-(BRV - BRV_{model})^2}{2\left(\frac{1}{6}(BRV_{up} - BRV_{btm})\right)^2} \right\} \tag{10}
\]

with

\[
BRV_{up} = BRV_{model} + (σ_{RSE}BRV_{model}) \tag{11}
\]

\[
BRV_{btm} = BRV_{model} - (σ_{RSE}BRV_{model}), \text{ with } \frac{ε_{IFC}}{ε} = 1 \tag{12}
\]

where the \(BRV_{model}\) represents the BRV prediction given by Equation (8), and where \(BRV_{up}\) and \(BRV_{btm}\) designate the upper and lower band values corresponding to one \(σ_{RSE}\) standard deviation.

One should note that the selected lower limit for \(\frac{ε_{IFC}}{ε} = 1\), as given by Equation (12), is the result of incipient fluidization conditions (IFC), in which there is a \(ε = 0.47\) uniform particle volume fraction throughout the bed. In fact, any bubble motion can only increase bed voidage, reducing the particle volume fraction, as a result. Thus, the maximum particle volume fraction achievable is the one obtained at IFC conditions, with this being the lowest \(\frac{ε_{IFC}}{ε}\) value from the PPM.

One should also consider that by using Equation (10), a probabilistic predictive model (PPM) can be established, with BAC distributions always complying with the condition of having a normalized area equal to one. As has been discussed before in previous publications by Torres Brauer [9], experimental evidence supports that measured BAC and BRV’s have normal distributions regardless of the experimental conditions. Because of this, the design of the PPM considers a normal distribution to generate simulated bubbles randomly.

The PPM proposed here will be employed in the upcoming sections of this manuscript, to predict single bubble velocities, for bubbles injected under incipient fluidization conditions, as defined by Torres Brauer et al. [19]. This PPM will be further evaluated in this manuscript, for BRV predictions in sand bubbling beds, with and without added biomass pellets.

5. Application of the PPM

Figure 4 reports the PPM density as a function of both the BAC and the BRV. Both BAC and BRV were calculated for single bubbles, as detected using the CREC-Optiprobe, in a sand bed at incipient fluidization conditions. On this basis, one can see that the bubble PPM density gives specific BAC levels with BRV density distributions. This confirms the critical need of establishing a PPM, as considered in the present study.

Furthermore, Figure 5 describes the probability distribution standard deviation as a function of the BAC, showing that this parameter increases progressively with bubble size. This demonstrates that flow randomness is limited for smaller bubbles, augmenting however, for larger bubbles.

Figure 6 reports the PPM given by Equation (9), with \(\frac{ε_{IFC}}{ε} = 1\), for both the lower and the upper BRV-BAC boundaries, and compares them with various technical literature correlations as reported in Section 1. Figure 6 shows that Equation (9), provides minimum and maximum BRV-BAC values, as set by the PPM, with these bands being \(±26\%\) of the average BRVs. These advisable BRV upper and lower limits account for the potential random variation of the particle volume fraction as well as for the BACs and the BRVs. One should note that predictions made by Davidson and Harrison [13], Wallis [14] and
Allahwala and Potter [17] fall within their suggested PPM range when no particle volume fraction correction is made. This is the case when $\frac{\text{circ}}{\epsilon} = 1$ in Equation (9).

![Figure 4](image-url)  
**Figure 4.** Probability density for the PPM for single bubbles injected at incipient fluidization conditions: (a) top view of the probability density plot; (b) isometric projection plot.

![Figure 5](image-url)  
**Figure 5.** Probability distribution standard deviation changes with the BAC.

![Figure 6](image-url)  
**Figure 6.** BRVs and BACs for various correlations available in the technical literature and for the proposed probabilistic predictive model (PPM). The PPM is represented with bands (minimum and maximum band values). Note: no particle volume fraction (pVolF) correction means that the term $\frac{\text{circ}}{\epsilon} = 1$ in Equation (9).

However, PPM bands are expanded, when the $\epsilon$ particle volume fraction becomes smaller than the IFC ($\frac{\text{circ}}{\epsilon} > 1$). At these conditions, both the Rowe and Yacono [16] and Rowe and Partridge [15] correlations fall within the bands of the PPM.
Furthermore, given the potential ability of the PPM to predict bubble behavior, including bubble flow randomness, the experimental data, as measured with CREC-Optiprobes and the HSCE model [19], were compared with the PPM results as shown in Figure 7. One can observe that the BRVs and the BACs obtained from the CREC-Optiprobes and the HSCE model provide reasonably congruent values, consistently falling within the PPM bands, as described by Equation (9). One can also notice that larger bubbles tend to fall outside the PPM range of predictions. This discrepancy is assigned to the influence of larger bubbles on local voidage volume fractions, and to the “double bubble effect”, with breaking bubbles forming a train and moving at a higher speed. This phenomenon is documented and discussed in [19].

![Figure 7](image7.png)

**Figure 7.** BRVs and BACs for single bubbles of all sizes, injected in the absence of biomass. Notes: (i) data points were obtained using the CREC-Optiprobes and the proposed HSCE model [19]; (ii) probabilistic predictive model (PPM) bands are set as proposed in the present study.

The proposed PPM can be applied further to sand beds with different concentrations of biomass. Figure 8 reports the behavior of single bubbles in a sand bed with 5 vol% of biomass, as detected using CREC-Optiprobes, and calculated by employing the HSCE model. In this case, one can notice an improvement in both the BAC size and BRV velocity predictions, with most of the injected bubbles falling within the proposed PPM bands. One can also notice that the bubbles with the added 5 vol% of biomass are now, on average, smaller. This behavior is attributed to the ability of the biomass pellets to act as bubble breakers, reducing the BACs of the bubbles and, consequently, their associated BRVs. It is worth mentioning that the proposed PPM equation does not have a specific term to address the presence or absence of biomass pellets, with the \( \frac{\text{BAC}}{\text{BRV}} \) ratio in Equation (9) accounting for the bed changes due to the added biomass.

![Figure 8](image8.png)

**Figure 8.** BRVs and BACs for single bubbles of all sizes, injected in the presence of 5 vol% biomass. Notes: (i) data points were obtained using the CREC-Optiprobes and the proposed HSCE model [19]; (ii) probabilistic predictive model (PPM) bands are set as proposed in the present study.
Figure 9 further reports the behavior of single bubbles in a sand bed with 10 vol% of biomass, as detected using the CREC-Optiprobex, and calculated by employing the HSCE model. One can see that the resulting bubbles are even smaller in this case, given the greater amount of biomass pellets in the bed, which act as bubble breakers. These bubbles all fall inside the set PPM bands.

Figure 9. BRVs and BACs for single bubbles of all sizes, injected in the presence of 10 vol% biomass. Notes: (i) data points were obtained using the CREC-Optiprobex and the proposed HSCE model [19]; (ii) the probabilistic predictive model (PPM) bands are set as proposed in the present study.

6. Probabilistic Predictive Model (PPM) for Sand Fluidized Bubbling Beds

The application of the PPM requires one to know the average volume fraction of the particles in the sand bed during measurements, as per Equation (9). Equation (9) relates the ratio between the known particle volume fraction of the bed, at incipient fluidization conditions (IFC), to the particle volume fraction, measured during a particular run.

In the previous section, while exploring the single bubble injection experiments, the particle volume fraction term in Equation (9) was considered to have a value of 1, since the bed was kept at incipient fluidization conditions.

\[
\left( \frac{\epsilon_{IFC}}{\epsilon} \right)^n = 1
\]

In the case of the bubbling bed, however, this is no longer true, and the particle volume fraction has to be calculated for each operational condition studied. To accomplish this, Equation (13) is proposed.

In fact, by using the CREC-Optiprobe data output, one can determine the signals of a time series, corresponding to either the absence of bubbles or the presence of them, using the “on” and the “off” time periods, respectively. As a result, one can compare the “on” cumulative times of the signal series, with the ones at incipient fluidization, defining a corrected value for the \( \epsilon_{IFC} \) parameter as follows:

\[
\epsilon = \epsilon_{IFC} \frac{t_{on}}{t_{tot}}
\]  
(13)

where the \( t_{on} \) is the total time with “positive (on)” CREC-Optiprobe signals (“absence of bubbles”), while the \( t_{tot} \) is the total time for the recorded cumulative “on” and “off” signals, during a run.

Thus, and on this basis, the particle volume fractions were determined experimentally, as shown in Table 1.

Following this, the PPM, as proposed via Equation (9), was considered for three sets of superficial gas velocities, with the sand bed in the bubbling regime and the bed free of biomass pellets. The selected superficial gas velocities were at 60, 70 and 80 SCFM airflows as shown in Figure 10a–c. These 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, respectively.
Table 1. Particle volume fractions for the five experimental runs studied. Note: Airflows are given in standard cubic feet per Minute (SCFM).

| Particle Volume Fraction | 0.438  |
|--------------------------|--------|
| 60 SCFM—0% Biomass       | 0.438  |
| 70 SCFM—0% Biomass       | 0.432  |
| 70 SCFM—25% Biomass      | 0.442  |
| 80 SCFM—0% Biomass       | 0.427  |
| 80 SCFM—25% Biomass      | 0.445  |

Following this, the PPM, as proposed via Equation (9), was considered for three sets of superficial gas velocities, with the sand bed in the bubbling regime and the bed free of biomass pellets. The selected superficial gas velocities were at 60, 70 and 80 SCFM airflows as shown in Figure 10a–c. These 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, respectively.

Figure 10 reports both the BRVs and BACs for bubbles measured in a bubbling regime without biomass, in a sand bed, under volumetric airflows of: (a) 60 SCFM; (b) 70 SCFM, and (c) 80 SCFM. Notes: (i) data points were obtained using CREC-Optiprobes and the proposed HSCE model [19]; (ii) the probabilistic predictive model (PPM) is reported with an orange band.

Table 2 also provides information about the bubbles that fall outside the proposed PPM band. It reports bubble number fractions of PPM overpredicted and underpredicted bubbles. One can thus notice that the fraction of overpredicted BACs corresponds to 2–8% of the total, while the fraction of underpredicted bubbles represents 15–16% of the total. Thus, in practice, the PPM overpredicted bubbles display BACs smaller than 5 cm, while the underpredicted bubbles have BACs larger than 5 cm. The reason for this discrepancy
is assigned to the influence of bed random effects in smaller bubbles and the “tunneling” effects in larger bubbles.

Figure 11 further reports the PPM bands when a 25 vol% of biomass pellets is loaded in the bed. Data reported correspond to 70 and 80 SCFM volumetric flows. One can again see, in this case, that the bubble fraction number falls within the PPM band is a 75–80% favorable range. The PPM overpredicted and underpredicted bubbles, as shown in Table 3, represent only 8–9% and 12–16%, respectively. As a result, one can conclude that the reported results set excellent prospects for BRV-BAC predictions, in bubbling sand fluidized beds with added biomass.

Table 2. Number of bubbles and bubble number fractions with the BRVs and the BACs within the PPM band and number of bubbles and bubble number fractions outside the PPM bands. Note: The sand bed is without biomass pellets.

| Experimental Run | Bubbles inside the PPM Prediction Band | Bubbles “below” the PPM Prediction Band | Bubbles “above” the PPM Prediction Band |
|------------------|--------------------------------------|----------------------------------------|----------------------------------------|
|                  | Bubbles | Fraction | Bubbles | Fraction | Bubbles | Fraction |
| 60 SCFM (Figure 10a) | 592 | 83% | 11 | 2% | 108 | 15% |
| 70 SCFM (Figure 11b) | 672 | 79% | 37 | 4% | 138 | 16% |
| 80 SCFM (Figure 10c) | 765 | 76% | 82 | 8% | 164 | 16% |

Figure 11. BRVs and BACs for bubbles measured in the bubbling regime, with 25 vol% biomass, in a sand bed, under volumetric airflows of: (a) 70 SCFM, and (b) 80 SCFM. Notes: (i) data points were obtained using the CREC-Optiprobes and the proposed HSCE model [19]; (ii) the probabilistic predictive model (PPM) is reported with an orange band.

Table 3. Bubble number and bubble number fractions with BRVs and BACs falling inside the PPM bands, as well as below and above the PPM bands. Note: The sand bed has 25 vol% biomass pellets.

| Experimental Run | Bubbles inside the Prediction Band | Bubbles “below” the Prediction Band | Bubbles “above” the Prediction Band |
|------------------|----------------------------------|------------------------------------|------------------------------------|
|                  | Bubbles | Fraction | Bubbles | Fraction | Bubbles | Fraction |
| 70 SCFM 25 vol% Biomass (Figure 11a) | 455 | 80% | 47 | 8% | 68 | 12% |
| 80 SCFM 25 vol% Biomass (Figure 11b) | 470 | 75% | 56 | 9% | 99 | 16% |

In summary and on the basis of the reported results, one can notice that the proposed PPM is able to effectively predict the BRV versus BAC values as a band of values, for sand fluidized beds with a single injected bubble, at incipient fluidization. One can also see that the PPM also applies to bubbly fluidized beds with and without loaded biomass pellets. It is anticipated that the proposed PPM will be of significant value for the design and the operation of sand fluidized beds for biomass gasification, where the BRV versus the BAC predictions are of critical importance.
7. Application of the PPM in a Fluidized Bed Reactor

The PPM can be used to predict the position, the BAC and the BRV of bubbles inside the fluidized bed, while providing a full 3D picture of the bubble axial and radial distributions. This information can be used later to determine the overall reactant conversion, and the product selectivity in fluidized bed reactors, while employing a two-phase model with a dense phase and a PPM bubble phase. Species balances can be established based on: (a) species molar flows with bubbles evolving in compliance with the PPM; (b) chemical species transformations including heterogenous and homogeneous reactions; and (c) chemical species transfer between phases via PPM bubble interfaces. Additional details about the PPM and its application to biomass gasifiers will be reported in a forthcoming article.

Furthermore, in order to establish the PPM as a valuable tool for fluidized bed reactor design and simulation, an original calculation method is proposed in the present study. This provides an “instantaneous 3D image” of the fluidized reactor, based on experimentally determined parameters, as previously explained in Section 6.

In addition, and as considered in the present study, this calculation method includes the random selection of bubbles sizes, conforming to the experimentally measured bubble size distribution. This calculation with bubble selection proceeds, until the experimentally observed bed expansion is reached.

Figure 12 provides a flow chart, describing the various calculation steps involved in the proposed method as follows:

1. Loading experimental parameters such as bed height, average gas volume fraction, minimum and maximum BACs. These parameters are discussed with more detail in Appendix A
2. Loading the PPM parameters $(\gamma, r, \varepsilon, \varepsilon_{IFC})$;
3. Calculating the $\Delta V$ volume of a hollow cylinder with a $r$ radius;
4. Randomly generating cylindrical coordinates $(r, \theta, z)$ and the BAC within anticipated ranges;
5. Calculating the BRVs using the PPM;
6. Calculating the $\varepsilon$ bed porosity in the considered $\Delta V$ volume;
7. Establishing if the calculated $\varepsilon$ value is larger than the anticipated $\varepsilon$ value;
8. If the answer is “yes”, the next step includes checking that the resulting “$\varepsilon$” also complies with being smaller than the anticipated $\varepsilon$, plus an allowed 2% deviation;
9. Alternatively, if the answer in (8) is “no”, one can proceed to 4), selecting another bubble;
10. Furthermore, if the answer in (8) is “no”, the calculation involves disregarding the bubble considered from further analysis and moving to step (4);
11. Next if the answer in (8) is positive, one should establish if this is the last $\Delta V$ control volume to be considered, with the entire bed radial geometry being covered. If the answer is “yes”, the calculation is complete. However, if the answer is “no”, the following calculation involves selecting a next $\Delta V$ and moving to step (4).

Furthermore, Figures 13–15, Tables 4–6, report three typical examples of 3D bed information at a selected time, using the bubble properties selection (BAC and BRV), described in Figure 12. These figures also provide information on the bubble positioning in the bed, for 60 SCFM, using the calculation method developed in the present study. This analysis can be repeated many times as required, to make it statistically meaningful.

In summary, if one applies the methodology of the PPM as described in the present study, one can conclude that the state of the bed, in terms of bubble flow, can be defined in terms of probabilistic-based parameters. For instance, if one applies the PPM to a fundamentally based fluidized bed chemical reactor simulation, with trustable kinetics, one can see that reactor performance indicators, such as reactant conversion and product selectivity, can only be defined via average parameters with their respective standard deviations, properly accounting for the intrinsic fluidized bed randomness. Thus, one can conclude that while the described PPM model is valuable for biomass sand fluidized gasifiers, adaptations may be required to account for biomass particle sizes and densities changes during gasification.
Figure 12. Description of various calculations steps involved in the application of the PPM.

Figure 13. Position of the calculated bubbles using the PPM developed in this study. Calculation 1 at 60 SCFM.
In summary, if one applies the methodology of the PPM as described in the present study, one can conclude that the state of the bed, in terms of bubble flow, can be defined in terms of probabilistic-based parameters. For instance, if one applies the PPM to a fundamentally based fluidized bed chemical reactor simulation, with trustable kinetics, one can see that reactor performance indicators, such as reactant conversion and product selectivity, can only be defined via average parameters with their respective standard deviations, properly accounting for the intrinsic fluidized bed randomness. Thus, one can conclude that while the described PPM model is valuable for biomass sand fluidized gasifiers, adaptations may be required to account for biomass particle sizes and densities changes during gasification.

### Table 6

| Bubble | BAC (m) | BRV (m/s) |
|--------|---------|-----------|
| 1      | 0.0934  | 0.9229    |
| 2      | 0.1455  | 1.1821    |
| 3      | 0.0791  | 0.7547    |
| 4      | 0.058   | 0.7213    |
| 5      | 0.1252  | 1.1538    |
| 6      | 0.093   | 1.0149    |
| 7      | 0.0525  | 0.8098    |
| 8      | 0.0339  | 0.5609    |
| 9      | 0.1003  | 0.9429    |
| 10     | 0.03    | 0.5453    |
| 11     | 0.1078  | 0.9175    |
| 12     | 0.0821  | 0.7734    |
| 13     | 0.1096  | 0.9417    |
| 14     | 0.0666  | 0.6428    |
| 15     | 0.0534  | 0.569     |
| 16     | 0.1355  | 0.8973    |

**Figure 14.** Position of the calculated bubbles using the PPM developed in this study. Calculation 2 at 60 SCFM.

**Figure 15.** Position of the calculated bubbles using the PPM developed in this study. Calculation 3 at 60 SCFM.

**Table 4.** Identification number for each bubble reported in Figure 13, along with size and velocity of each bubble.
Table 5. Identification number for each bubble reported in Figure 14, along with size and velocity of each bubble.

| Bubble | BAC (m) | BRV (m/s) |
|--------|---------|-----------|
| 1      | 0.0726  | 0.7471    |
| 2      | 0.0378  | 0.5237    |
| 3      | 0.1092  | 1.0258    |
| 4      | 0.1309  | 1.0012    |
| 5      | 0.1353  | 1.1331    |
| 6      | 0.0478  | 0.707     |
| 7      | 0.1085  | 1.0421    |
| 8      | 0.1424  | 0.9757    |
| 9      | 0.0379  | 0.5071    |
| 10     | 0.0964  | 0.7618    |
| 11     | 0.0833  | 0.664     |
| 12     | 0.0518  | 0.6094    |
| 13     | 0.0838  | 0.659     |

Table 6. Identification number for each bubble reported in Figure 15, along with size and velocity of each bubble.

| Bubble | BAC (m) | BRV (m/s) |
|--------|---------|-----------|
| 1      | 0.0934  | 0.9229    |
| 2      | 0.1455  | 1.1821    |
| 3      | 0.0791  | 0.7547    |
| 4      | 0.058   | 0.7213    |
| 5      | 0.1252  | 1.1538    |
| 6      | 0.093   | 1.0149    |
| 7      | 0.0525  | 0.8098    |
| 8      | 0.0339  | 0.5609    |
| 9      | 0.1003  | 0.9429    |
| 10     | 0.03    | 0.5453    |
| 11     | 0.1078  | 0.9175    |
| 12     | 0.0821  | 0.7734    |
| 13     | 0.1096  | 0.9417    |
| 14     | 0.0666  | 0.6428    |
| 15     | 0.0534  | 0.569     |
| 16     | 0.1355  | 0.8973    |

8. Conclusions
(a) It is confirmed that bubble flow description in sand fluidized beds requires a probabilistic predictive model (PPM), given the intrinsic bubble flow randomness;
(b) It is shown that the proposed PPM overcomes the limitations of deterministic correlations, used to describe bubble dynamics, in high-density sand beds of Type B particles of the Geldart classification;
(c) It is proven that the proposed PPM can describe the BAC-BRV relationship using minimum and maximum values, and a PPM band. This PPM applies to a wide range of operating conditions;
(d) It is shown that the proposed PPM can be considered for single bubbles, injected into a bed, at incipient fluidization, and to bubbly beds, with and without loaded biomass pellets;
(e) It is proven that the calculation method developed in the present study can be used to identify the position of bubbles, their BACs and BRVs and their associated randomness;
(f) It is shown that the proposed PPM analysis can be repeated as many times as desired, allowing the prediction of reactant conversion and product selectivity as statistically based performance parameters.

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**Nomenclature**

**Symbols**

| Symbol | Dimension | Description |
|--------|-----------|-------------|
| \(D_{\text{bed}}\) | \(\text{m}\) | Diameter of the bed |
| \(d_{\text{beq}}\) | \(\text{m}\) | Equivalent bubble diameter |
| \(g\) | \(\text{m/s}^2\) | Standard acceleration due to gravity (9.8 m/s²) |
| \(n\) | dimensionless | Empirical order in the PPM |
| \(t_{\text{on}}\) | \(\text{s}\) | Amount of time the sensor registers the laser as “ON” (no bubble condition) in the CREC-Optiprobe System |
| \(t_{\text{tot}}\) | \(\text{s}\) | Total amount of time registered in the experiment regardless of laser status in the CREC-Optiprobe system |

**Greek Symbols**

| Symbol | Dimensionless | Description |
|--------|---------------|-------------|
| \(\epsilon\) | | Particle volume fraction |
| \(\epsilon_{\text{IFC}}\) | | Particle volume fraction at incipient fluidization conditions |
| \(\Omega\) | | Empirical probabilistic coefficient in the PPM |
| \(\gamma\) | | Empirical deterministic coefficient in the predictive models |
| \(\sigma_{\text{RSE}}\) | | Standard deviation of the relative signed errors |

**Acronyms**

| Acronym | Description |
|---------|-------------|
| BAC | Bubble axial chord |
| BM | Biomass |
| BM vol\% | Volume percentage of biomass pellets content in the bed |
| BRV | Bubble rise velocity |
| BRV\(_{\text{model}}\) | Bubble rise velocity calculated by the proposed model without the probabilistic component (deterministic approach) |
| CREC | Chemical reaction engineering center |
| FR | Bubble frontal radius |
| HESC | Hybrid experiment-spherical cap |
| PPM | Probabilistic predictive model |
| Syngas | Synthesis gas |
| SCFM | Standard cubic feet per minute |
| vol\% | Volume percentage |

**Appendix A**

The model described in Figure 12 mentions experimental parameters to be loaded in the software. These parameters are:

(a) Bed height;
(b) Average particle volume fraction measured in the bed for each measurement point;
(c) Minimum Bac;
(d) Maximum Bac.

The bed height was directly measured from the experimental setup. This parameter provides the upper limit for the position (z) that a bubble can occupy in the bed without breaking due to reaching the surface.

The average particle volume fraction on each measurement point was determined from experimental data. After recording and analyzing more than 1000 bubbles, the total “ON” time of the sensor of the CREC-Optiprobe system was considered as “Empty of sand” time. Considering the total time of the experiment, one can obtain a particle volume fraction averaged over time for a particular point in the reactor. Assuming that this particle volume fraction should be maintained over time in the column that represents the bubble path, and considering the cylindrical symmetry, this average volume fraction was applied...
to a cylindrical ring called control volume. This data is useful to know how many bubbles can be simulated in a particular Control volume before exceeding the correct number and as a consequence decreasing the particle volume fraction beyond the control parameter.

Finally, minimum and maximum BAC was determined from experimental data series for each measurement point. These parameters are the lower and upper limit for the random BAC generation.

As an example, Table A1 shows the parameters used for the simulation of bubbles under a 60 SCFM airflow.

**Table A1.** Example of the parameters used for the simulation of bubbles at air flow conditions of 60 SCFM obtained from experimental analysis.

| Measurement Point | Bed Height (m) | Average pVol Fraction | Minimum BAC (m) | Maximum BAC (m) |
|-------------------|----------------|-----------------------|-----------------|-----------------|
| 1                 | 0.4            | 0.443                 | 0.03            | 0.147           |
| 2                 | 0.439          |                       |                 |                 |
| 3                 | 0.438          |                       |                 |                 |
| 4                 | 0.453          |                       |                 |                 |
| 5                 | 0.467          |                       |                 |                 |
| 6                 | 0.47           |                       |                 |                 |
| 7                 | 0.47           |                       |                 |                 |
| 8                 | 0.47           |                       |                 |                 |

References

1. Göransson, K.; Söderlind, U.; He, J.; Zhang, W. Review of syngas production via biomass DFBGs. *Renew. Sustain. Energy Rev.* 2011, 15, 482–492. [CrossRef]

2. Boerrigter, H.; Rauch, R. Syngas Production and Utilisation, Chapter 10. In *Handbook Biomass Gasification*; BTG: Enschede, The Netherlands, 2005; pp. 211–230.

3. Torres, L.; Urquina, L.; Hernandez, N.; de Lasa, H. Costa Rica Coffee Pulp (Broza) Gasification. A Stoichiometric-Chemical Equilibrium Model. In Proceedings of the 5th International Congress on Green Process Engineering (GPE 2016), Mont Tremblant, QC, Canada, 19–24 June 2016; Available online: http://dc.engconfintl.org/gpe2016/57 (accessed on 6 September 2017).

4. Savuto, E.; Di Carlo, A.; Steele, A.; Heidenreich, S.; Gallucci, K.; Rapagnà, S. Syngas conditioning by ceramic filter candles filled with catalyst pellets and placed inside the freeboard of a fluidized bed steam gasifier. *Fuel Process. Technol.* 2019, 191, 44–53. [CrossRef]

5. Rapagnà, S.; Gallucci, K.; Di Marcello, M.; Foscolo, P.; Nacken, M.; Heidenreich, S.; Matt, M. First Al₂O₃ based catalytic filter candles operating in the fluidized bed gasifier freeboard. *Fuel* 2012, 97, 718–724. [CrossRef]

6. De Filippis, P.; Scarsella, M.; De Caprariis, B.; Uccellari, R. Biomass Gasification Plant and Syngas Clean-up System. *Energy Procedia* 2015, 75, 240–245. [CrossRef]

7. Di Giuliano, A.; Foscolo, P.U.; Di Carlo, A.; Steele, A.; Gallucci, K. Kinetic Characterization of Tar Reforming on Commercial Ni-Catalyst Pellets Used for In Situ Syngas Cleaning in Biomass Gasification: Experiments and Simulations under Process Conditions. *Ind. Eng. Chem. Res.* 2021, 60, 6421–6434. [CrossRef] [PubMed]

8. Geldart, D. The effect of particle size and size distribution on the behaviour of gas-fluidised beds. *Powder Technol.* 1972, 6, 201–215. [CrossRef]

9. Torres Brauer, N. *Bubble Dynamics in a Sand Fluidized Bed in the Presence of Biomass Pellets*; Western University: London, ON, Canada, 2020.

10. Davies, R.M.; Taylor, G.I. The mechanics of large bubbles rising through extended liquids and through liquids in tubes. *Proc. R. Soc. Lond. Ser. A Math. Phys. Sci.* 1950, 200, 375–390. [CrossRef]

11. Kunii, D.; Levenspiel, O. Bubbling Bed Model. Model for Flow of Gas through a Fluidized Bed. *Ind. Eng. Chem. Fundam.* 1968, 7, 446–452. [CrossRef]

12. Kunii, D.; Levenspiel, O. *Fluidisation Engineering*; Butterworth-Heinemann: Boston, MA, USA, 1991.

13. Davidson, J.F.; Harrison, D. *Fluidised Particles*; Cambridge University Press: Cambridge, UK, 1963.

14. Wallis, G.B. *One Dimensional Two-Phase Flow*; McGraw-Hill: New York, NY, USA, 1969.

15. Rowe, P.; Partridge, B. An x-ray study of bubbles in fluidised beds. *Chem. Eng. Res. Des.* 1997, 75, S116–S134. [CrossRef]

16. Rowe, P.N.; Yacono, C.X.R. The Bubbling Behaviour of Fine Powders When Fluidised. *Chem. Eng. Sci.* 1976, 31, 1179–1192. [CrossRef]

17. Allahwala, S.A.; Potter, O.E. Rise Velocity Equation for Isolated Bubbles and for Isolated Slugs in Fluidized Beds. *Ind. Eng. Chem. Fundam.* 1979, 18, 112–116. [CrossRef]

18. Karimipour, S.; Pugsley, T. A critical evaluation of literature correlations for predicting bubble size and velocity in gas–solid fluidized beds. *Powder Technol.* 2011, 205, 1–14. [CrossRef]
19. Brauer, N.T.; Rosales, B.S.; De Lasa, H. Single-Bubble Dynamics in a Dense Phase Fluidized Sand Bed Biomass Gasification Environment. *Ind. Eng. Chem. Res.* **2020**, *59*, 5601–5614. [CrossRef]
20. Fotovat, F.; Abbasi, A.; Spiteri, R.J.; De Lasa, H.; Chaouki, J. A CPFD model for a bubbly biomass–sand fluidized bed. *Powder Technol.* **2015**, *275*, 39–50. [CrossRef]
21. Fotovat, F.; Chaouki, J.; Bergthorson, J. The effect of biomass particles on the gas distribution and dilute phase characteristics of sand–biomass mixtures fluidized in the bubbling regime. *Chem. Eng. Sci.* **2013**, *102*, 129–138. [CrossRef]
22. De Lasa, H.; Lee, S.L.P.; Bergougnou, M. Bubble measurement in three-phase fluidized beds using a u-shaped optical fiber. *Can. J. Chem. Eng.* **1984**, *62*, 165–169. [CrossRef]
23. Rüdisüli, M.; Schildhauer, T.J.; Biollaz, S.M.; Van Ommen, J.R. Bubble characterization in a fluidized bed by means of optical probes. *Int. J. Multiph. Flow* **2012**, *41*, 56–67. [CrossRef]