NUMERICAL STUDY OF THE DYNAMIC FLOW BEHAVIOUR IN A LABORATORY SCALE BUBBLE COLUMN OPERATING UNDER HOMOGENEOUS AND HETEROGENEOUS REGIME

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Introduction

• Bubble column reactors (BCR) are widely used in processes that require continuous contact between two phases, gas and liquid, due to their excellent heat and mass transfer characteristics.

• simplicity in its construction and operation, small floor area and absence of moving parts are the main advantage of this equipment.

• bubbles columns show a complex flow....→ transition between the flow regime..... homogeneous to heterogeneous...
Introduction

• In this sense....

• **experimental** and **numerical** study of bubble column behavior is very important ... provides an **useful** and **essential** information for suitable **design** and **operation** to scale-up of this type of equipment.

• Its requires a **detailed** description of the **bubble characteristics, mass and heat transfer parameters, chemical kinetics**.... and are **highly** dependent on the local **dynamics of the multiphase flow**....

• in this way, the **numerical simulation** of the gas-liquid flow using computational fluid dynamics (CFD) has become an **essential tool**;
Introduction

• ... the main goal of the present work is to use a “low cost” CFD methodology that is capable to predict the two-phase flow in homogeneous and heterogeneous regime....
Experimental methodology

• Provides an **useful and essential data** to validate the numerical methodology

• Experimental Unit of Bubble Column (EU-BC)
  – cylindrical bubble column
  – constructed in acrylic material
  – dimensions: $D = 150 \text{ mm}$ and $H = 1000 \text{ mm}$
  – the gas distributor (bottom of the column), dispersing plate which has a porous mesh area of $24.75 \text{ cm}^2$
  – superficial velocity of gas phase ranging from $0.05$ to $0.10 \text{ m s}^{-1}$

Liquid velocity and gas global volumetric fraction
Experimental methodology

- **PIV** to determine the liquid axial velocity.... 425 seconds measured in each case at 0.5m from the gas sparger

- **Hydrostatic pressure difference** to determine the global gas volume fraction.... 10 minutes measured in each case ...

\[
\bar{v}_l = \frac{\sum_{n=1}^{N} v_l}{N}
\]

\[
\bar{\varepsilon}_g = \frac{1}{\rho_l - \rho_g} \left( \rho_l - \frac{\bar{p}_1 - \bar{p}_2}{g \Delta h} \right)
\]

**Experimental apparatus:** (1) bubble column, (2) gas distributor, (3 and 4) temperature sensors, (5) pressure sensor, (6) air flow meter, (7) control valve, (8) compressed air, (9) control valve, (10) controlled gas flow, (11) central data communication, (12) management, acquisition and control.
Numerical methodology

• The bubble column flow is composed by three phases: **liquid**, "small" bubbles and "large" bubbles ... methodology also adopted by Krishna et al. (1999)

• **Eulerian description** was used for each of these phases, by:

\[
\frac{\partial}{\partial t} (f_k \rho_k v_k) + \nabla \cdot (f_k \rho_k v_k v_k) = 0, \quad T_k^{\text{eff}} = -\mu_k^{\text{eff}} \left[ \nabla v_k + (\nabla v_k)^T \right]
\]

\[
\frac{\partial}{\partial t} (f_k \rho_k v_k) + \nabla \cdot \left( f_k \rho_k v_k v_k + f_k T_k^{\text{eff}} \right) = -f_k \nabla p_k + \sum_{k \neq j}^{np} F_{kj} + \rho_k f_k g
\]

\[
\sum_{k=1}^{np} f_k = 1
\]

\[
\sum_{k \neq j}^{np} F_{kj} = F_{gl} = -F_{lg} = F_{gl}^D + F_{gl}^L + F_{gl}^{VM} + \cdots
\]

• Transient simulations were carried using **ANSYS CFX 13.0** and all the simulations were performed by using **2D axis-symmetry**
Numerical methodology

- The **Interphase** momentum transfer describes the **interaction** at the interface between the phases. Due to the small effect on the numerical results, the virtual mass force was neglected. The drag force model was proposed by Krishna and Ellenberger (1996):

\[
F_{g-l}^L = C_L f_g \rho_g (v_g - v_l) \times \nabla \times v_l
\]

\[
F_{g-l}^D = \beta_{gl} A_g^p (v_g - v_l)
\]

\[
A_g^p = \frac{3 f_g}{2 d_g}
\]

\[
\beta_{gl} = \frac{1}{2} \rho_l C_D |v_g - v_l|
\]

\[
C_D = \frac{4}{3} \frac{\rho_l - \rho_g}{\rho_l} g d_{b,i} \frac{1}{V_{b,i}^2}
\]

\[
V_{b,small} = 1.53 \left( \frac{\sigma_g}{\rho_l} \right)^{0.25}
\]

\[
V_{b,small} = 0.71 \left( g d_{b,large} \right)^{0.5} (SF) (AF)
\]

\[
d_{b,large} = \gamma (U - U_{trans})^\delta
\]

\[
AF = \alpha + \beta (U - U_{trans})
\]

\[
\gamma = 0.069 \quad \delta = 0.376 \quad \alpha = 2.73 \quad \beta = 4.505
\]

... while "small" and "large" bubbles **do not** interact to each other ....
Numerical methodology

• **30 seconds** of real time are simulated with a time step of **0.005 seconds**...

• **atmospheric pressure** at the outlet, **non-slip** condition for the **liquid** and **free slip** to the **gas phase** on the walls. The "bubbles" enter with a **normal uniform speed**. The **volume fraction at inlet** of the “bubbles” phase is given by:

\[
U < U_{\text{trans}} \rightarrow \text{homogeneous regime} \rightarrow f_{\text{small}} = 1 \quad \text{and} \quad f_{\text{large}} = 0
\]

\[
U > U_{\text{trans}} \rightarrow \text{heterogeneous regime} \rightarrow f_{\text{small}} = \frac{U_{\text{trans}}}{U} \quad \text{and} \quad f_{\text{large}} = \frac{(U - U_{\text{trans}})}{U}
\]
The geometry, mesh and boundary conditions are given by:

<table>
<thead>
<tr>
<th>Boundary</th>
<th>Condition</th>
<th>( f_1 )</th>
<th>( f_{\text{small}} )</th>
<th>( f_{\text{large}} )</th>
</tr>
</thead>
</table>
| **Inlet** | \( v_{x, i} = 0, v_{z, i} = \frac{Q}{A}, v_{y, i} = 0 \); \( v_{y} = 0, v_{z} = 0; \)
| \( k = 1.5 (|v_y| L)^2 \), \( \varepsilon = C_{\mu} k^{1.5} L \). | \( 1 - (f_{\text{small}} + f_{\text{large}}) \) | \( \frac{U_{\text{trans}}}{U} \) | \( \frac{(U - U_{\text{trans}})}{U} \) |
| **Outlet** | \( \frac{d v_{x, i}}{d \eta}, \frac{d v_{y, i}}{d \eta}, \frac{d v_{z, i}}{d \eta} = 0 \), \( \frac{d v_{x, i}}{d \xi}, \frac{d v_{y, i}}{d \xi}, \frac{d v_{z, i}}{d \xi} = 0 \), \( \frac{d k}{d \eta} = \frac{d \varepsilon}{d \eta} = 0, P = P_{\text{ref}} \), \( \frac{d v_{x, i}}{d \eta} = \frac{d v_{y, i}}{d \eta} = \frac{d v_{z, i}}{d \eta} = 0 \), | \( \frac{d f_{\text{small}}}{d \eta} = 0 \) | \( \frac{d f_{\text{large}}}{d \eta} = 0 \) |
| **Wall** | \( v_{i} = 0, v_{j} = 0, v_{k} = 0 \), \( \frac{d k}{d \eta} = \frac{d \varepsilon}{d \eta} = 0 \). | \( \frac{d f_{i}}{d \xi} = 0 \) | \( \frac{d f_{\text{small}}}{d \xi} = 0 \) | \( \frac{d f_{\text{large}}}{d \xi} = 0 \) |
| **Symmetry** | \( \frac{d k}{d \eta} = \frac{d \varepsilon}{d \eta} = \frac{d P}{d \eta} = \frac{d v_{y, i}}{d \eta} \), \( \frac{d f_{i}}{d \eta} = 0 \), \( \frac{d f_{\text{small}}}{d \eta} = 0 \), \( \frac{d f_{\text{large}}}{d \eta} = 0 \) | \( \xi \) Orthogonal wall direction, \( \eta \) normal direction. |

\( I \) turbulence intensity (5%), \( L \) length scale.
Numerical methodology

- A high-order interpolation scheme was used for the hydrodynamics equations and upwind for the turbulence equations. The time discretization is performed in a fully implicit first order approximation.

- Comparison between the numerical and experimental data was made in the same positions of the measurements ...

<table>
<thead>
<tr>
<th>Variable evaluated</th>
<th>Modified parameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>Global gas volume fraction</td>
<td>gas superficial velocity - 0.00509 to 0.10 m s(^{-1})</td>
</tr>
<tr>
<td>Liquid axial mean velocity</td>
<td>gas superficial velocity - 0.00509, 0.01276, 0.01786 and 0.02808 m s(^{-1})</td>
</tr>
</tbody>
</table>
Results – Experimental Data

- Experimental results: global gas volume fraction and regime transition identification
Results – Experimental Data

- Experimental results: mean axial **liquid velocity**, that provides useful parameter to design, operation and scale-up bubble column equipment...

**parabolic shape**, the traditional overall recirculating flow with an **up-flow** in center axis and **down-flow** close the wall. In the **homogeneous** regime has the form of a flattened parabolic profile. **Increasing gas flow rate**, the parabolic shape is accentuated showing greater magnitude for the upward and downward liquid velocity.

!!!!!! For $U > 0.02808 \text{ m s}^{-1}$ it wasn’t possible to get reliable data using PIV.
Results – Numerical Results and Model Validation

• Comparison between numerical and experimental data to the **global gas volumetric fraction**

It can be seen that the simulations reproduce the global gas holdup trends with the increasing of gas velocity.

The model reproduces the characteristic of **change slope profile**, as like the experimental data....
Results – Numerical Results and Model Validation

- **Effects of gas flow at numerical experiments...**

...under **homogeneous** regime, velocity profiles have a **flatter parabolic shape**, only “small” bubbles is considered.

In **heterogeneous regime**, parabolic profiles have a more **inclined shape**, is given by to the presence of “large” bubble, this **rise and form clusters in the central regions of the column**, this bubbles have a high speed, lead to a more pronounced speed in the liquid phase....
Results – Numerical Results and Model Validation

- Velocity profile of numerical bubbles phase observed for all three regimes.

for "small" bubble phase velocity profiles are more homogeneous along the radius of the column for all regimes, due the lift force....

for "large" bubble phase a velocity peak is viewed in central regions, with velocities from two to three times larger than "small" bubble phase...
Results – Numerical Results and Model Validation

- Measured profiles of time average axial velocities with the corresponding simulation results for the height of 0.5 m under **homogeneous** regime.
Results – Numerical Results and Model Validation

- Measured profiles of time average axial velocities with the corresponding simulation results for the height of 0.5 m at in transition heterogeneous regime.

\[ U = 0.01786 \text{ ms}^{-1} \text{ at 0.5m to gas distributor} \]

\[ U = 0.02808 \text{ ms}^{-1} \text{ at 0.5m to gas distributor} \]
Conclusions

- It was observed that the liquid velocity phase is heavily affected by changing superficial velocity of the gas phase (U), and therefore the operation regime of the column.

- The simulations are validated with experimental data for global gas holdup and liquid-phase axial velocities. The time-averaged variables is well predicted as shown by the comparison of measured radial profiles of the mean values.

- This “low cost” CFD methodology is capable to simulate a bubble column operating at homogeneous and heterogeneous regime.
References

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