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ABSTRACT

The present work focuses on the development of a novel computational code able to predict with a reasonable level of accuracy the bubble behavior in gas fluidized beds with minimum computational demands. The code simulates the bubble chaotic rise motion and coalescence along bed height via simple lagrangian tracking of bubbles. An original empirical model for the assessment of bubble-bubble interactions is developed. The code is used to simulate a lab-scale unit in bubbling and slugging mode. On this basis, fast simulations are performed to successfully predict bubble population and fluxes within the bed.

The main aim of this code is to be embedded within CAPE codes for the process simulation. The model adopted by the code is also well suited for multi-scale modeling approach since physical parameters can be obtained from both experimental data or CFD simulation.

Preliminary results of the simulations, in terms of distributions for bubble size and number as well as local hold up values, are compared with relevant experimental data.

Keywords: modeling; discrete bubble model; numerical simulation; 2D;

INTRODUCTION

Modeling of fluidized bed equipment is an open task, mainly because of the complexity of the physical phenomena involved. Different classes of model have been developed in the past. Empirical models are those where simple correlation are developed on the basis of experimental data. Such models, very simple to use, often offer poor reliability for design and scale up, being normally highly dependent on the geometry and the scale of the experimental set-up adopted for the experiments. Semi-Fundamental models are those developed at a length scale smaller than the whole system, but larger than particles, where mass, momentum and energy balances (coupled with the suitable closure relations to model fluid turbulence, among others) are solved numerically in order to predict the complex behaviour of the system. These models (Eulerian-Eulerian models, Eulerian-Lagrangian models) are actually the most used, since reliable predictions can be obtained even if large computational times are required. The reliability of these models is strictly related to the closure relations adopted. Fundamental models directly solve microscopic mass, momentum and energy balances, without the need for any closure relation. Fluid turbulence and relevant interactions with particles are directly simulated. These models are not actually available to simulate even lab-scale systems, due to the enormous computational time required.

A recently developed class of models in the field of fluidization studies is that of the so called Discrete Bubble Models, in which bubble motion through a continuous emulsion phase is modeled and solved, including at the present state of development bubble motion and coalescence (1-4). This class of models is mainly aimed in setting up very simple and computationally inexpensive simulation of bubble population within fluidized beds. In this paper an extremely simplified model for bubble-to-bubble interaction description is reported in order to allow very fast computation of bubble population. The aim of this contribution is the preliminary development of a mathematical model for the description of bubbling fluidized bed behaviour, operating at an intermediate scale of detail, able to simulate the chaotic behaviour of fluidized beds in a simplest way with respect to semi-fundamental models. The model developed is then compared with relevant experimental data (5)

MATHEMATICAL MODELLING

Discrete Bubble models treats each bubble individually, following its trajectory along its path through the bed. The basic of DBM were described elsewhere (1-4). In order to solve bubble motion through the bed, different physical phenomena should be taken in account, each one affecting the history of each bubble. In the following some of the most relevant works are reported:

1. Emulsion phase modeling: a Eulerian description of the emulsion phase can be implemented within the code (3) to increase the predictivity of the model, but this greatly increases the computational effort. On the other hand, it was previously shown that sufficiently accurate simulation can be ran without solving solids motion, provided that the relevant effect on bubble motion is somehow modeled (1-2,4). In this contribution, a stationary emulsion phase is assumed.
2. Single bubble motion: the velocity of a single bubble rising through a fluidized bed was thoroughly investigated in the past (6-7), with different correlations developed where bubble vertical velocity mainly depends on bubble diameter. The equations adopted are thoroughly discussed in he following
3. Bubble to bubble interactions: in the presence of a bubble swarm, it is well accepted that the trajectory of each bubble is strongly influenced by the vicinity of other rising bubbles; the passage of a bubble in a fluidized bed is in fact associated with a perturbation of the pressure field with respect to the repose condition (8). The pressure perturbation located in the wake region of the bed is responsible for the capture motion of bubbles and thus is one of the principal cause of coalescence (9). A simplified mathematical model based on the net effect of neighboring bubbles on the bubble trajectory was already adopted in the past (1) for computer simulation through DBM. A suitably developed model is here proposed and discussed in the following.
4. Bubble coalescence; the coalescence phenomenon has been extensively studied, being the principal cause of bubble enlargement along bed height (9-11). In the case of DBM, it is possible to follow different approaches (delayed *vs* non-delayed coalescence, 1) in order to take in account for the shape of bubbles. The volume of the bubble formed after coalescence may also have a smaller volume than the coalescing bubbles in certain conditions (12). In this contribution, non-delayed coalescence is assumed.

5. Bubble splitting. Bubbles rising in fluidized bed may also undergo splitting, eventually leading to measurable maximum stable size before the onset of slugging regimes (8). No splitting bubbles are considered hare.
6. In addition, some modeling is needed to assess the effect of distributor design, wall conditions and freeboard region. The relevant equations adopted are discussed in the "Boundary conditions" section of this paper.

Bubble main rise velocity: The principal bubble motion is assumed to be the rising motion from the distributor to the bed surface. The bubble rise velocity has been extensively studied, and several literature works (6,10) agree in stating that bubble rise velocity mainly depends on bubble equivalent diameter:

$$\frac{u_b}{\sqrt{g d_b}} = \begin{cases} 0.71 \rightarrow \text{Davidson (1963)} \\ 0.8 \div 1 \rightarrow \text{Shen (2004)} \end{cases} \tag{1}$$

This correlation represents the main velocity for the bubbles. The use of a mechanicistic law is compatible with the chaotic behaviour of fluidized beds, if it is assumed the presence of perturbation to this motion, due to the interaction between non contacting bubbles.

Bubble coalescence: each bubble is assumed to have constant volume in absence of bubble interactions (this consideration implies that the gas permeating from the bubble to the emulsion phase is equalized by the gas permeating into the bubble from the emulsion phase). Bubbles conserve volume through bubble coalescence or splitting (even if some papers show that bubble volume is not conserved during coalescence under some circumstances, 12). In the simplified model proposed, bubble coalescence occurs if the distance between two bubble becomes minor or equal to the half sum of the diameters (non-delayed coalescence, 1), giving rise to a bubble whose volume equals the sum of the volumes of the coalescing bubbles. Moreover, it is assumed that the bubble centroid of the new bubble will lie along the segment connecting the original centroids, at a coordinate given by:

$$\vec{x}_{b,new} = \frac{V_{b,1}}{V_{b,1}+V_{b,2}}\vec{x}_{b,1} + \frac{V_{b,2}}{V_{b,1}+V_{b,2}}\vec{x}_{b,2} \tag{2}$$

Weak bubble interactions: bubble vertical trajectory is generally modified by the presence of neighboring bubbles, which induce lateral and vertical acceleration in the bubble motion. To account for this phenomenon, it is worth reminding that each bubble generates a pressure perturbation located in the proximity of its wake region (8). The part of the perturbation falling out of the bubble (i.e. in the emulsion phase) would be able to drive the other bubbles toward coalescence.

In this work, a simplified model of the pressure driven attraction generated by the *i-th* bubble on the *j-th* bubble is proposed (Pressure Driven Velocity Perturbation, *PDVP*). It is physically expected that the attraction intensity would fall rapidly toward zero if the distance between the bubbles is increased, and that larger bubbles will give rise to more pronounced attraction field with respect to smaller bubbles. In particular, the attraction intensity will depend on the mass of both bubbles. On these basis, the proposed field assumes the form:

$$\Delta P_{i,j} = -K_1 \frac{V_{b,i} V_{b,j}}{\sqrt{(x_i - x_j)^2 + (y_i - y_j - 0.3 d_{b,i})^2}} \qquad (3)$$

Where K_1 is an empirical constant. Since bubbles are considered as spherical, and the center of the generated field being located at about $0.2d_b$ above the bottom of the bubble (approximately near the wake region), the singularity of the field falls inside the bubble itself. The pressure field accelerates all other bubbles towards the bubble wake region, as it is effectively possible to observe in bubbling fluidized beds. This generates the expression reported in Eqn.3 for the effective bubble distance in pressure perturbation calculation. In the simplified model proposed (induced mean velocity is assumed instead of induced acceleration), the velocity induced in a second bubble by the pressure perturbation generated by the first bubble is proportional to the pressure gradient and is inversely proportional to the mass of the second bubble:

$$\frac{\partial \vec{x_j}}{\partial t} = -K_2 \frac{\nabla(\Delta P_{i,j})}{V_{b,j}} \qquad (4)$$

Where K_2 is an empirical constant. Moreover, if N bubbles are present, the effects of the field generated by all bubbles except the *j-th* bubble have to be considered as acting on the *j-th* bubble:

$$\frac{\partial \vec{x_j}}{\partial t} = -\frac{K_2}{V_{b,j}} \nabla\left(\sum_N \Delta P_{i,j}\right) \qquad (5)$$

It is worth noting that the empirical constants K_1 and K_2 are presented as separate constants for the sake of clarity, but they can be condensed in a single empirical constant. Notably, the trajectory of each bubble depends on the position and volume of all other bubbles within the bed.

In the present contribution, the emulsion phase is treated as a stationary continuum, and no splitting mechanism is considered.

NUMERICAL SIMULATION

The computational domain have a simple geometry, exactly equal to the height and the width of the experimental set-up (H = 36cm, W = 18cm, t = 1.5cm, d_p = 212-250 mm, U = 18-27 cm/s; further details are given in 5).

Boundary conditions: Upper side of the bed is considered the bubble exit: all bubbles having a vertical coordinate greater than the height of the bed are not still considered into the computational domain. No particular conditions are needed at the lateral walls of the bed, since the *PDVD* generally directs bubbles towards the center of the bed, therefore preventing that bubbles unphysically exit through lateral walls, provided that a sufficiently small time steps is adopted. The distributor, placed at the bottom of the bed, is modeled in order to generate bubbles obeying the *TPM*. In particular, as a first approximation, the whole gas flow exceeding the minimum fluidization velocity results in visible bubble flow. The excess gas flow is equally divided to the N_c holes of the distributor. The lift off time of the bubble is reached when the gas area of the bubble reaches a critical value A_0.

This kind of arrangement gives high level of symmetry in the bed, thus generating banal numerical solution of the problem. In order to make visible the full chaotic behavior in simulation, the position of bubbles are slightly randomized in both vertical and horizontal position (the displacements are an order of magnitude inferior to the bubble diameters). As expected, this randomization will lead to full chaotic bubble motion.

The numerical simulation consists in the solution of the position of all bubbles in the bed by adopting a first order finite difference. The motion of each bubble is computed by firstly imposing the main displacement derived by Eqn. 1, and then computing the *PDVP* dependent displacements as computed by Eqn. 5. After the *PDVP* driven displacements are computed, the bubble coalescence logical condition is checked. It is worth noting that since no surface tension exists in fluidized beds at the separation layer between bubbles and emulsion phase, the coalescence step is not a rate determining one. The same observation is reported in the paper by Darton (9), in which is found that bubbles capture motion is the rate determining step.

The results of the simulation of 60 seconds real time can be obtained in few second with desktop PC Dell Inspiron 530S dual core.

RESULTS

The behaviour of the simulated fluid bed have been analyzed firstly in a qualitative fashion, by putting the numerical results in form of graphical maps.

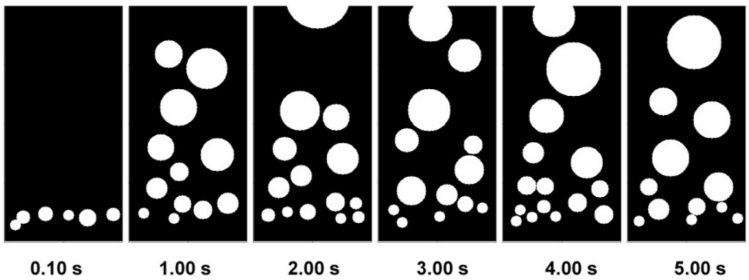
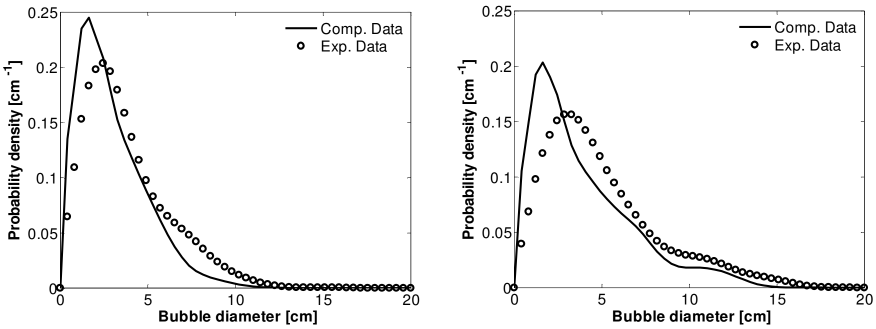


Figure 1: Graphical representation of simulated bubbles at U = 18 cm/s.

In Fig.1, a sequence of frames thus obtained is reported. The qualitative analysis show that the bubbles follow a chaotic behavior, without reaching stable configuration, in perfect agreement with experimental observation. Smallest bubbles are not reproduced in the snapshot for the sake of meaningful visual representation. The bubbles appear to uniformly form at the distributor and move toward the center of the bed. Along their path, bubbles coalesce, thus forming larger bubbles that move towards the bed exit. It is possible to observe a clear decrease of bubble number with the distance above the distributor and a significant bubble enlargement, as physically expected.

The qualitative observations made by visual analysis of the snapshots is therefore not sufficient for the validation of the results. A quantitative validation can be easily performed by comparing bubble size and position data with relevant experimental data from a previous work (5) where full details about the experimental set-up and the image analysis technique can be found.

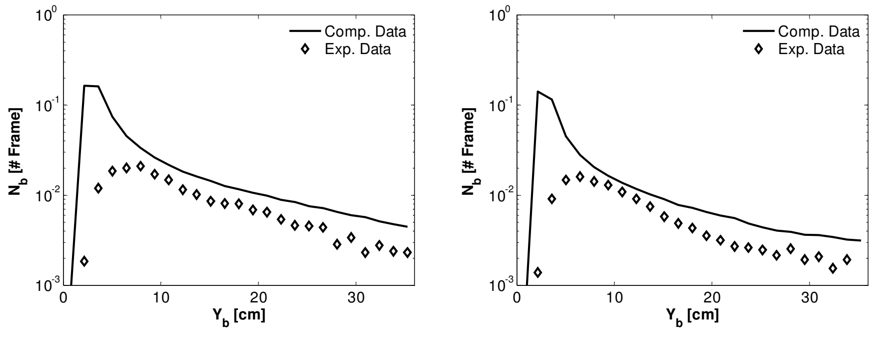
To assess the ability of the code in correctly simulating bubble sizes, the simulated Bubble Sizes Distributions (*BSD*) were computed and reported in Fig.2 in form of probability density functions together with relevant experimental data (5). A characteristic positively skewed distribution is found in all cases as physically expected. The code is also able to correctly predict the broadening of the BSD while increasing inlet gas velocity.



(a) (b)

Figure 2. Comparison between experimental and simulated data on Bubble Size Distribution within the bed (3a: U = 18 cm/s; 3b: U = 27 cm/s).

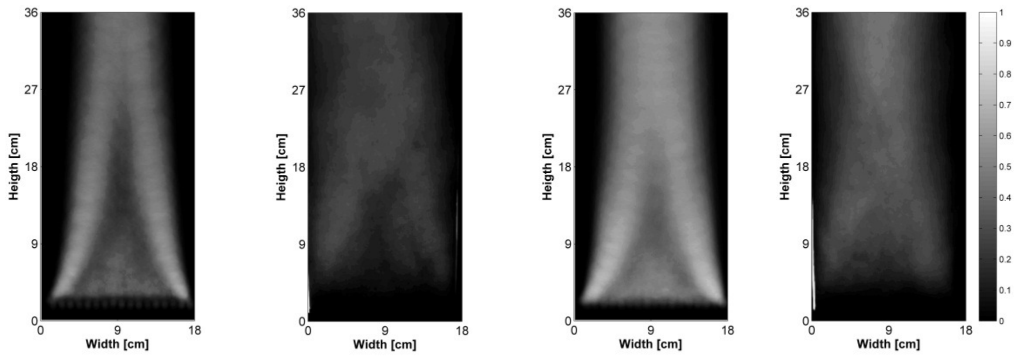
In order to validate the code for the prediction of net coalescence rate, it is useful to use the computation of the time-averaged bubble density as a function of distance along bed height. It is easy to show that a linear decay rate of bubble density is found in a semi-logarithmic plot when a first order bubble number decay rate is assumed (13). The computational data reported in Fig.3 clearly follow a linear decay, as physically expected. It is worth noting the excellent agreement between computational and experimental data, in the prediction of both slope of the linear decay rate and value of bubble density function.



(a) (b)

Figure 3. Comparison between experimental and simulated data on Bubble Number Distribution within the bed (4a: U = 18 cm/s; 4b: U = 27 cm/s.)

In Fig.4, the analysis of computational time averaged bubble phase hold-up allows the visual observation of preferential bubble paths along the bed, with a typical reverse-Y shaped pattern starting near the bottom of the bed and developing in the upper regions of the bed. The reverse-Y shaped pattern is due to the coalescence-driven bubble dynamics prevailing after bubble nucleation in the proximity of the distributor in the intermediate region of the bed. The comparison of computational maps (Figs. 4a, 4c) with relevant experimental bubble phase hold-up maps (Figs. 4b, 4d) highlights an overestimation of local hold-up, but the shape appears to be sufficiently well predicted. In particular, the overall hold up values in experimental cases were found to be 0.16 and 0.20 at U=0.18 m/s and 0.27 m/s respectively, while the relevant simulated data were in equal to 0.23 and 0.32 respectively. It is worth noting that this effect can be ascribed to the effect of threshold value in experimental bubble measurements (5) or, on the other hand, to some of the simplifying hypotheses of the adopted model such as (i) bubble constant volume through coalescence or (ii) gas troughflow absence. The sensitivity of the model to these hypotheses should be carefully checked, and this is one of the main objectives of future works.



(a) U=0.18m/s, comp; (b) U=0.18m/s, exp; (c) U=0.27m/s, comp; (d) U=0.27m/s, exp;

Figure 4. Comparison between experimental and simulated data on Local Bubble hold up. Colorbar data refers to time-averaged local hold up values.

CONCLUSIONS

In this work, a full-in-house developed code has been used to simulate in a Lagrangian fashion the behaviour of a bubbling fluidized bed. The model implemented in the code makes use of literature correlations and an original Pressure Driven Velocity Perturbation model, resulting in the prediction of the bubble patterns along bed height. A simple coalescence model has been used in order to predict bubble enlargement. The results obtained for the case of 2D simulations are compared with experimental data obtained by a purposely built 2D lab scale gas fluidized bed. The agreement of model predictions with experimental data appears satisfactory.

The Lagrangian simulation thus performed allowed the direct quantification of the relevance of the physical phenomena in bubbling fluidized beds, such as the fundamental role of inter-bubble interactions in determining bubble behaviour.

Further developments are expected with the implementation of bubble break-up models.

NOTATION

- A_0; Bubble area at the distributor;
- d_b; bubble equivalent diameter;
- g; acceleration due to gravity;
- K_1, K_2; model constants for PDVP;
- N_c; number of holes at the distributor;
- $P_{i,j}$; pressure driven attraction between generic bubbles;
- U; gas superficial velocity;
- u_b; bubble rise velocity;
- V_b; bubble volume;
- x_b; bubble centroid coordinate;

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