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CFD SIMULATION OF BINARY FLUIDIZED MIXTURES: EFFECTS OF RESTITUTION COEFFICIENT AND SPATIAL DISCRETIZATION METHODS

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ABSTRACT

This work focuses on the CFD simulation of fluidized bidisperse solid particles with same density and different size. We successfully predicted the minimum superficial gas velocity required to steadily fluidize the particles by employing a second-order upwind spatial discretization method and a non-ideal value of the restitution coefficient.

INTRODUCTION

Gas-solid fluidization is a widespread technology in many chemical and physical processes. Examples are freezing and mixing, or industrial processes involving solid-catalyzed reactions (1). The efficiency of fluidized systems relies on the enhanced gas-solid contact and heat and mass transfer. The bed hydrodynamic behavior determines whether a polydisperse powder mixes or segregates. Bubbles simultaneously induce particle mixing and segregation. In consequence, the solid axial profile throughout the bed under steady state conditions - being the result of the equilibrium between the two phenomena - depends on how vigorous the bubbling is (2). It is a general rule to classify the particles that accumulate at the top and bottom of the bed as flotsam and jetsam, respectively.

An extensive literature is available on the experimental characterization of mixing and segregation of polydisperse mixtures (3, 4, 5, 6). Even though experimental studies give a deeper insight into the fluidized mixture behavior, they are highly dependent on the system analyzed. So, one should couple experimental results with modeling to support the design of new systems.

To design industrial-size fluidized bed units, one needs accurate mathematical models that: i) integrate the experimental results in a theoretical framework and ii) are able to support scale-up and optimization of the apparatus. The advent of high performance computers allows to use Computational Fluid Dynamics (CFD) to simulate and predict the dynamics of fluidized beds. During the last years, the effects of set-up options, physical parameters, mathematical models, constitutive equations and numerical schemes on the mixing and segregation behavior of bidisperse mixtures have become a subject extensively studied in the literature (7, 8, 9, 10). Nevertheless, several issues are still open. In particular, the dynamics of segregation as well as the gas superficial velocity at the regime transitions are not very well predicted (11).

The present contribution is part of a wide project aiming at characterizing and simulating binary fluidized mixtures. As a first step, the study focused on the fluidization of a binary mixture of particles characterized by equal density (~2500 kg/m^3) and different size (500 μm and 125 μm diameter for jetsam and flotsam, respectively). This system was experimentally characterized by Marzocchella et al. (12). The average jetsam mass fraction in the bed was set at ω_1=0.5 and the bed was initially perfectly mixed. The minimum superficial gas velocity necessary to steadily fluidize and fully mix the powder, u*, was equal to 0.10 m/s. If the gas velocity u is greater than u*, the bed vigorously bubbles and the convective particle flow induced by the bubbles prevents axial segregation. The system was simulated by Mazzei et al. (11). Even though their simulations well reproduced the phenomenology of segregation if u<u*, they overestimated the minimum gas velocity required to steadily fluidize and fully mix the bed.

GOALS OF THIS WORK

The present work moves the study of Mazzei et al. (11) one step further. The CFD simulations address the following issues:

- Why u* was overestimated?
- How do spatial discretization schemes influence the steady-state jetsam segregation profiles and the bubble volume fraction?
- Does the restitution coefficient affect the bed dynamics?

To answer these questions, we focused on the role of physical parameters and numerical options. The study regarded:

1. Spatial discretization methods: first-order upwind scheme (FUS) and second-order upwind scheme (SUS). In the FUS, cell-face quantities are determined by assuming that the cell-center values of any field variable represent cell-averages that hold throughout the entire cells. In the SUS, higher-order accuracy at cell faces is attained with a Taylor expansion of the variable about the cell centroid. Both schemes introduce numerical diffusion, which is the phenomenon that smooths out the gradients of all variables. However, SUS is less diffusive than the FUS. More in details, only for the volume fraction equation, we employed a particular type of second order discretization, the QUICK method.
2. Restitution coefficient. This coefficient, denoted as e, is: 1 when particle collisions are ideal; less than 1 when a part of the kinetic energy is lost during the collisions.

This study aimed to optimize the value of the restitution coefficient and to find the best numerical options to correctly predict the minimum gas velocity at which the powder, previously described, mixed completely.

NUMERICAL TECHNIQUES

Simulations were carried out using the commercial CFD package Fluent 12 until the system attained steady-state conditions. The simulated domain is two-dimensional and the effect of the front and back walls are neglected. The vessel is 1 m high and its width is 0.12 m. The bed material occupies 40% of the vessel. Walls are ‘no-slip’ for both the gas and solid phases. The pressure at the outlet is set to 10^5 Pa. To describe the fluidized powder behavior, we solved the averaged equations of motion for the fluid phase and the two solid phases (jetsam and flotsam), and the energy balance for the granular temperatures. The full mathematical model with closure relations can be found in Mazzei et al. (11). Fluent uses a multifluid approach to solve the averaged equation of motions. We used the pressure-based solver, which is recommended for low-speed incompressible flows.

Coroneo et al. (13) studied the accuracy of the computational method used. They introduced a global parameter that takes into account not only the grid size and the time step (as the Courant number), but also the operating conditions of the bed. We chose a time step of 10^{-3} and an uniform mesh size of 5 mm because the value of 2.5 of the global parameter (calculated for our case), following the approach of Coroneo et al. (13), allows an average absolute error less than 5%. Therefore, there was no need of taking in consideration smaller grid sizes and time steps. A maximum of 200 iterations was sufficient for the flow variable to converge to the specified threshold of 10^{-5}. Under relaxation factors of 0.20 were adopted for all the variables. We investigated the powder behavior for gas velocities of 0.10, 0.12, 0.14 m/s, setting the restitution coefficient at 0.60, 0.70, 0.80, 0.90, 0.99.

Simulation results were reported in terms of bubble volume fraction, denoted as δ, spatial profiles of fluid volume fraction and jetsam concentration profiles for different values of the restitution coefficient and of the superficial gas velocity at steady-state. We calculated δ as the ratio between the volume occupied by bubbles and the entire volume occupied by the bed of particles. Furthermore, we divided the bed in six horizontal layers of equal height and calculated the average values of jetsam volume fraction within each layer, assigning them to the heights of the layer upper boundaries. As simulated fluidized beds have different heights, we normalized the height of each layer with respect to the overall bed height, H_{max}, to compare the results. Bubble volume fraction and jetsam concentration profiles are time averaged values between 15 s and 30 s whereas the spatial profiles of fluid volume fraction statistically represent steady conditions after 15 s.

RESULTS

First-order upwind scheme

If a first-order spatial discretization scheme was chosen, the bubble volume fraction slightly increased with the restitution coefficient (Figure 1).

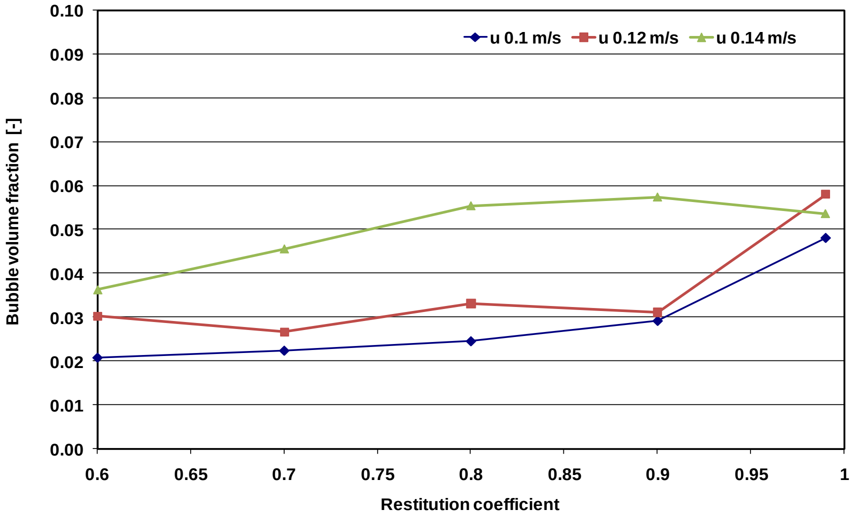

Figure 1. Stationary bubble volume fraction profiles as a function of restitution coefficient for different fluid velocities. FUS.

Figure 2 reports snapshots of the fluid volume fraction for three values of the superficial gas velocity under steady-state conditions. The results refer to a simulation carried out setting the restitution coefficient at 0.7. The results obtained for different values of e did not differ significantly from those reported in Figure 2. The voidage inside the bubbles was far less than unity and the bubble size was smaller than that experimentally observed (14) in fully bubbling beds.

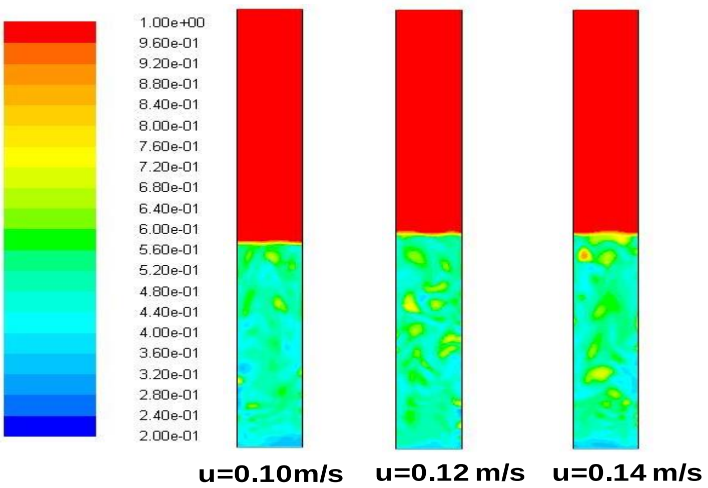

Figure 2. Fluid volume fraction spatial profiles, at steady state, for superficial fluid velocities of 0.10, 0.12 and 0.14 m/s and a restitution coefficient of 0.70. FUS.

Jetsam concentration profiles along the axis of the bed for different values of the restitution coefficient and for a superficial velocity of 0.10 m/s, compared with experimental results (12), are reported in Figure 3. The results did not change significantly when u was changed within the investigated interval.

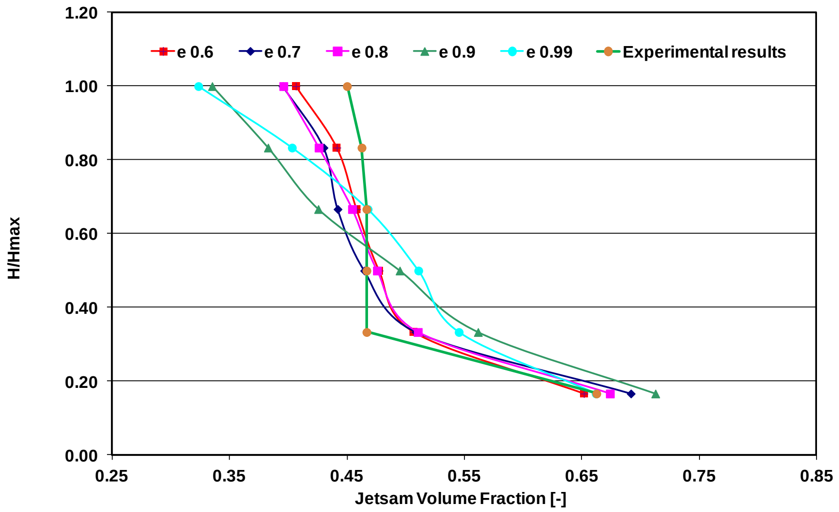

Figure 3. Stationary axial profiles of average jetsam volume fraction as a function of restitution coefficient. The superficial fluid velocity is 0.10 m/s. FUS. Comparison with the experimental results.

The jetsam profiles in Figure 3, are characterized by segregation of flotsam and jetsam at the top and the bottom of the bed, respectively.

The analysis of the results suggests that the discretization schemes adopted were unable to capture the relevant phenomenology of the binary fluidized bed. In particular, we observed that:

- the value of δ was too low (Figure 1) to have physical sense: it never exceeded 6%.
- At steady-state bubbles were few and small, not occupying a significant volume of the fluid bed and their boundaries not being clearly defined (Figure 2).
- Mixing was not achieved because the small bubbles did not promote convective particle flow.
- The restitution coefficient had a marginal effect on the bed dynamics.

Second-order upwind scheme

Figure 4 reports the bubble volume fraction as a function of the restitution coefficient for several values of the superficial gas velocity, for simulations carried out with the second-order spatial discretization scheme. Except for e=0.99, the bubble volume is quite constant with the restitution coefficient, ranging between ~10 % for u=0.10 m/s and ~16% for u=0.14 m/s. The bubble fraction assessed for simulations carried out by adopting the SUS increased almost ten times when compared to those assessed by adopting the FUS.

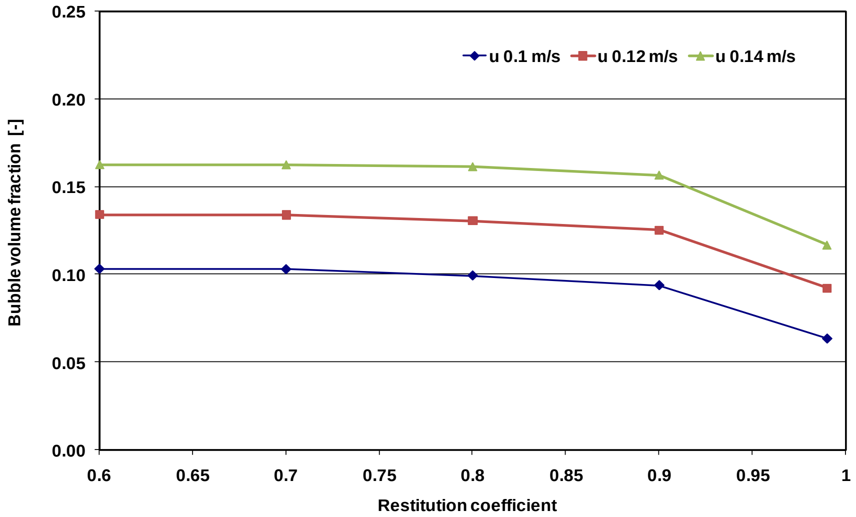

Figure 4. Stationary bubble volume fraction profiles as a function of restitution coefficient for different fluid velocities. SUS.

The analysis of the snapshots referred to steady states established at different superficial gas velocities (Figure 5) highlights that bubbles were larger and their boundaries were clearly defined. In this case, bubbles occupied a significant part of the bed volume and therefore they affected more strongly the particle flow.

The void fraction inside the bubbles approached unity and the bubble size agreed with experimental values reported for fully bubbling beds (14). Bubble motion let jetsam float freely in the upper part of the bed, while transferring flotsam to the bottom.

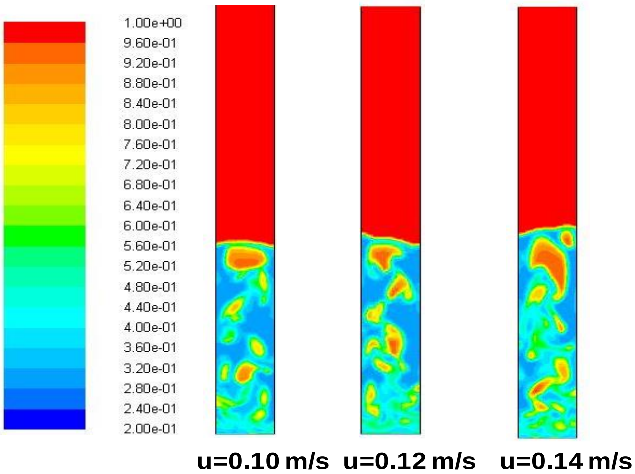

Figure 5. Fluid volume fraction spatial profiles, at steady state, for superficial fluid velocities of 0.10, 0.12 and 0.14 m/s and a restitution coefficient of 0.70. SUS.

Figure 6 reports the jetsam concentration profiles assessed along the bed axis for different values of the restitution coefficient and for u=0.10 m/s, compared with experimental results (12). At higher superficial velocities results were very similar to those reported in Figure 6. The restitution coefficient did not strongly influence the bed dynamics: the profiles for all values of this coefficient were vertical, except for the bottom part of the bed and for the value of e=0.99.

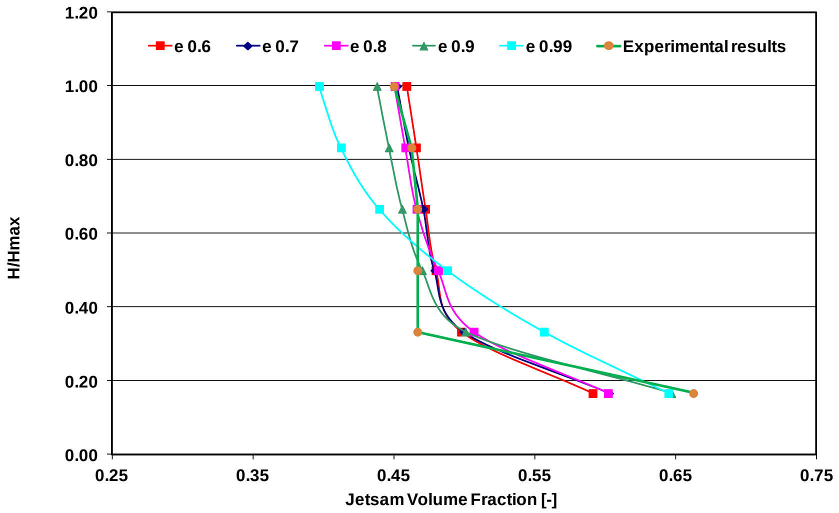

Figure 6. Stationary axial profiles of average jetsam volume fraction as a function of restitution coefficient. The superficial fluid velocity is 0.10 m/s. SUS. Comparison with the experimental results.

All together, the binary mixtures resulted better mixed when SUS was adopted.

CONCLUSIONS

This work aimed to simulate the behavior of a fluidized bidisperse mixture of solids to further the study of Mazzei et al. (11), where the minimum superficial gas velocity to attain full mixing was overestimated. The focus was on the influence of the restitution coefficient and of the spatial discretization schemes on the solids dynamics. Main remarks are reported below.

- If u>u* the bed bubbled, the vigorous bubbles promoting convective flow of particles; thus, at equilibrium the powder was fully mixed. Numerically, bubbles are discontinuities in the emulsion phase, and since numerical diffusion smooths out the gradients of all variables, CFD may generate unreal and small bubbles. This was the case of FUS. Being FUS more diffusive than SUS, simulation carried out adopting FUS did not correctly reproduce the vigorous bubbles observed experimentally. Accordingly, the jetsam concentration profiles simulated with FUS showed an unexpected segregation and that was the reason why Mazzei et al. (11) predicted an overestimated velocity of ~ 60 cm/s to obtain full mixing. Under bubbling conditions, SUS correctly simulated the bed dynamics, yielding correct jetsam concentration profiles and vigorous bubbling. In this case, u* was not overestimated and well matched the experimental results of Marzocchella et al. (12).
- The restitution coefficient did not strongly influence the bed dynamics except for the value e=0.99.

NOTATION

e Restitution coefficient

H_{max} Time averaged overall bed height
u superficial velocity magnitude (m/s)
u* minimum superficial velocity at which particle mixture fully fluidizes (m/s)
δ bubble volume fraction
ω_i mass fraction i th particle phase on fluid-free basis

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