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Pattern formation in fluidized beds as a tool for model validation: A two-fluid model based study

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ABSTRACT

Computational fluid dynamics (CFD) models have been broadly used during the last twenty years to engineer and understand fluidized beds. Nevertheless, there is some controversy about the rigor of their current validation methodologies (Powder Technol. 139 (2004), 99). A robust tool to determine whether or not a model reproduces—let alone, can predict—the dynamics of a fluidized bed is still missing. This is especially relevant for the validation of the fluid-particle closures that are emerging with the help of direct numerical simulation.
More than a decade ago, it was demonstrated experimentally that regular patterns emerge in pulsed fluidized beds under certain experimental conditions. These patterns are not a singular feature of the dynamics, such as average bubble size or bed expansion, but form as a result of a precise coupling between multi-scale physical phenomena. Remarkably, CFD has not been able, so far, to reproduce the experimental bubble patterns convincingly. In this work, we want to bring to the attention of the fluidization community the power of pattern formation in fluidized beds as a tool for model validation. As a proof of concept, we apply this validation test to two-fluid models. Our two-fluid simulations reproduce bubble properties reasonably well, but fail to reproduce the experimentally witnessed patterns, suggesting that the physics of the fluidized state are not correctly captured by this approach, under any of its common implementations.

1. Introduction

Gas–solid fluidized beds are widely used in industrial processes where good heat and mass transfer are of paramount importance. The mixing and transport properties of these reactors originate from non-linear physical phenomena occurring at multiple spatio-temporal scales, resulting in complex dynamics [1] that greatly complicate fluidized bed control and scale-up [2].

Computational fluid dynamics (CFD) has been broadly used during the last twenty years to facilitate the engineering and understanding of fluidization processes [2–6]. Two main approaches can be distinguished: two-fluid models (Eulerian–Eulerian) and discrete particle models (Eulerian–Lagrangian). In two-fluid models, both the gas and particle phases are treated mathematically as interpenetrating continua, and one solves for the local solids concentration instead of the particle trajectories [3]. Averaging the instantaneous equations in a suitable way allows one to use a coarser mesh and longer time steps, decreasing the computational effort at the cost of introducing unknowns into the governing equations. The model must be completed by defining closure laws—topological, constitutive, and transfer laws— which can be derived from empirical information, phenomenological models and micromechanical theories. Two-fluid models are broadly used in the fluidization field since they can simulate systems up to 1 m or more in a reasonable amount of time. However, they are deemed more useful for predicting qualitative trends than absolute values mainly due to the inaccuracies of the closure laws [2].

Discrete particle models apply the discrete treatment to a dispersed phase, which is resolved by tracking particles individually following Newton's laws of motion. These models can be divided into discrete element models (DEM) and direct numerical simulations (DNS). In DEM, the mesh size of the Eulerian grid is at least one order of magnitude larger than the particle size [5]. Particles are treated as point sources and sinks of momentum, requiring the use of closures to solve the gas–particle interaction. This approach can simulate systems up to 0.1 m and help to unravel the influence of particle–particle, gas–particle, and particle–wall interactions in the formation and mixing of heterogeneous flow structures. On the contrary, the size of the Eulerian grid in DNS is at least one order of magnitude smaller than the particle size [7,8]. Gas–particle interactions are resolved by imposing a stick boundary condition at the surface of a particle. DNS is the only approach that does not require the implementation of closures, because it does not involve averaging. Although it is the most computationally expensive

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simulation technique, one of its appeals is that it can help to develop the closure laws for fluid–particle interactions necessary to simulate larger systems [6].

CFD validation has progressed in parallel to model development, and is subject to intense discussion [9–11]. Simple models based on empirical correlations are considered helpful when they are able to predict an experimental phenomenon under a limited range of physical conditions. More fundamental models, including the main physical mechanisms, such as the models included in commercial CFD packages, are expected to represent the process over a broad range of conditions in a more reliable way. A large variety of physical systems and models complicate a systematization of the validation procedure. In addition, the substantiation test that a model must pass to be considered valid often depends on the expectations for the model and, sometimes, even on the researchers' interests [9,11]. Grace and Taghipour [11] provided several guidelines for CFD validation in an effort to avoid the excessive claims that are common in the literature. Examples are: covering a broader range of conditions, performing proper error analysis, and seeking expert opinion to determine whether or not there is agreement between the experimental and modeled phenomenon. Some of these guidelines can be fulfilled with good experimental and numerical practices, whereas other ones remain inherently subjective. There is no consensus on how broad the experimental space must be, what phenomena the model must explain to be considered fully validated, or when simulated and experimental traits can be considered in “reasonable agreement”. Models are typically tested by comparing the experimental and theoretical bubble properties [12–16], void fraction [17,18], particle velocity [13,19–22], segregation [18], time-averaged solid/gas volume fractions [13], bed expansion [13,14], pressure fluctuations [23–25], and mass flux profiles [26]. These are different manifestations of the system dynamics that are, ultimately, what the model should be able to reproduce.

More than a decade ago, Coppens et al. [27,28] demonstrated experimentally that a pulsated gas flow could induce the formation of regular bubble patterns in gas–solid fluidized beds. In quasi-2D beds, that is, thin in one horizontal dimension, bubbles rise forming hexagonal configurations (Fig. 1), whereas, in shallow 3D beds, regular patterns form on the top surface resembling those observed in vibrated granular media [29,30]. Independently of the bed geometry, experimental bubble patterns are sub-harmonic; bubbles alternate their positions in each pulse and the pattern is repeated after two pulses. Pattern formation in fluidized beds has remained highly unexplored and is not understood yet, although preliminary studies point at phase locking (synchronization) as a possible mechanism [27]. The theory of dynamical synchronization is too vast to be described here in detail, but the main idea is that a periodic external force can stabilize certain states of chaotic dynamics, represented by orbits in a strange attractor [31]. Hence, synchronization depends on the properties of the external force and attractor topology, such as local trajectories, and phase dynamics. Simulating synchronization in a chaotic fluidized bed requires a model that captures at least the main features of the attractor, which are intimately related to the multi-scale dynamics of the underlying physical system.

Few attempts have been made in this direction. Kawaguchi et al. [32] studied pulsed fluidization using DEM. They reported that pulsation frequencies of 4–5 Hz induced regularity in the bubble behavior for Geldart B particles. A row of two large bubbles at fixed positions was stably formed in each pulse; however, the sub-harmonic, alternating behavior that is characteristic of the experimental patterns was not observed. [33] also conducted DEM of fluidization of Geldart B particles, finding that frequencies of 5–10 Hz increased the regularity of the bubble dynamics. However, their results are far from the clear experimental patterns, something the authors attribute to the thin bed—one particle diameter—and insufficient simulation time.

It is remarkable that CFD simulations have not been able to convincingly reproduce, so far, the experimental bubble patterns. Patterns are not one feature of the dynamics, but emerge from the coupling between dynamics occurring at multiple spatio-temporal scales [34]. To reproduce the patterns, the model must capture the underlying physics of the fluidized state in a proper manner. This allows to validate CFD models based on their ability to reproduce the experimentally witnessed regular patterns. In addition, regular patterns (bubbles patterns in quasi-2D beds or surface patterns on 3D beds) are easy to identify visually, preventing the artifacts introduced by many experimental and analysis techniques, and facilitating the comparison between the modeled and experimental system. Although the synchronization phenomenon in fluidized beds is a promising tool for CFD validation, it has been largely ignored by the fluidization community, so far.

In this work, we show the power of pattern formation for CFD validation using two-fluid models as a case study. Two-fluid models are extensively used in the fluidization field [2,3,13,17,22], and their low computational effort compared to other approaches makes them a natural first choice for our purpose. More complex CFD models, such as DEM, will also be tested in the future.

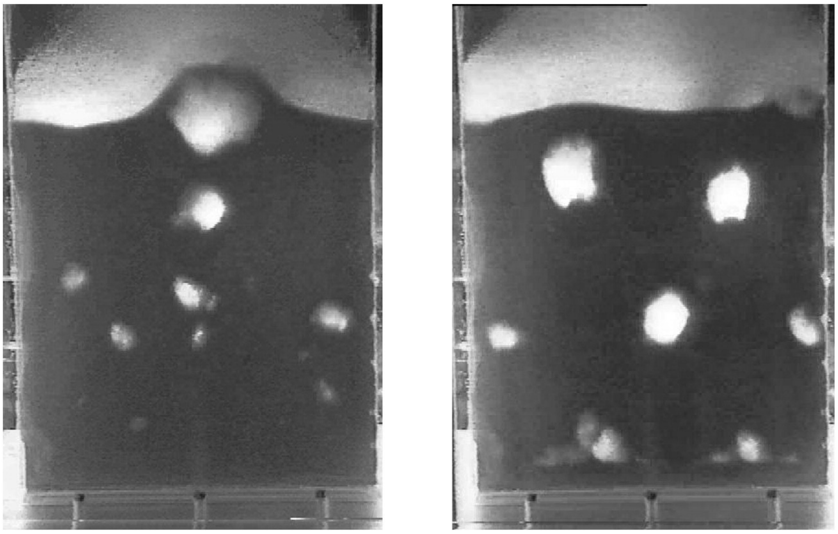

Fig. 1. Quasi-2D bed of sand fluidized with air at $u_0/u_{\mathrm{mf}} = 1.3$ (left) and $u_0/u_{\mathrm{mf}} = 1.3 + 0.5\sin(2\pi 4t)$ (right). The hexagonal bubble configuration generated by the oscillating flow is evident. The movies of these snapshots are included in the Supplementary Material.