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# A comparative study of different CFD-codes for numerical simulation of gas–solid fluidized bed hydrodynamics

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ABSTRACT

The hydrodynamics of a gas–solid fluidized bed reactor were studied numerically. Computational two-dimensional results from open source software packages `MFIX` and `OpenFOAM`, and those obtained from the commercial software package `Fluent` were discussed and compared with numerical and experimental data existing in the literature. The gas–solid flow was simulated applying the multifluid Eulerian–Eulerian model, where the solid phase is treated as a continuum. The solid-phase properties were calculated by using the kinetic theory of granular flow. Momentum exchange coefficients were calculated using the Gidaspow and Syamlal–O'Brien drag functions. Pressure drop and bed expansion ratio predicted by the simulations were in relatively close agreement with benchmark numerical and experimental data sets in the bubbling regime. Contrary to the `OpenFOAM` predictions, computations with `MFIX` and `Fluent` predicted instantaneous and time-average local voidage and velocity profiles which are comparable with results from the literature.



## 1. Introduction

Fluidized bed combustion and gasification of coal and biomass is used for power-generation in different industries like plant operations, chemical, pharmaceutical and mineral industries. Because of their complex flow behavior and the many solid particle interactions, the numerical modeling of fluidized bed reactors is very challenging. Good process control of an inherently unstable process such as fluidization is fundamental for an adequate use of this technology. Information on fluidization can be found in books, e.g. by Gidaspow (1994), and on general particle–fluid flow in books by Crowe, Sommerfeld, and Tsuji (1998) and Michaelides (2006).

The fundamental problem encountered in modeling hydrodynamics of a gas–solid fluidized bed is the two phases motion with unknown and transient interface. In conformity to Gilbertson and Yates (1996) the interaction is understood only for a limited range of conditions. Two main approaches exist to apply CFD modeling to gas–solid hydrodynamics. The Eulerian–Lagrangian approach is a discrete method based on molecular dynamics in which explicit motion of the interface is not modeled. In this method the continuous phase is modeled using an Eulerian framework and the trajectories of each solid particle is simulated in a Lagrangian framework. Therefore, this approach is efficient only for flows containing a low volume fraction of solid particles. The second approach for modeling gas–solid flows is the multi-fluid or Eulerian–Eulerian model, also called granular flow model. This continuous approach is based on continuum mechanics treating the two phases as interpenetrating continua and can be applied to multiphase flow processes containing large volume fractions of dispersed phase. Due to the discrete character of the underlying process, this approach requires extensive modeling efforts to provide a model involving a continuum associated with the dispersed phase particles. While some of the correlations used in the models remain to be empirical or semi-empirical, application of CFD to model fluidized bed hydrodynamics continues to develop. The models and their parameters must be validated against experimental measurements obtained at similar scale and configurations. Some of the challenges with respect to CFD model validation for gas–solid fluidized beds have been reviewed by Grace and Taghipour (2004). A review of discrete particle models used for the flow phenomena study prevailing in fluidized beds was given by Deen, Van Sint Annaland, Van der Hoef, and Kuipers (2007).

Hydrodynamic studies of two-dimensional fluidized bed columns (see Fig. 1) are often used to analyze and explore bubble properties and to provide qualitative viewing of fluidization characteristics such as growing and coalescence. The motion of bubbles and particles in fluidization phenomena are greatly

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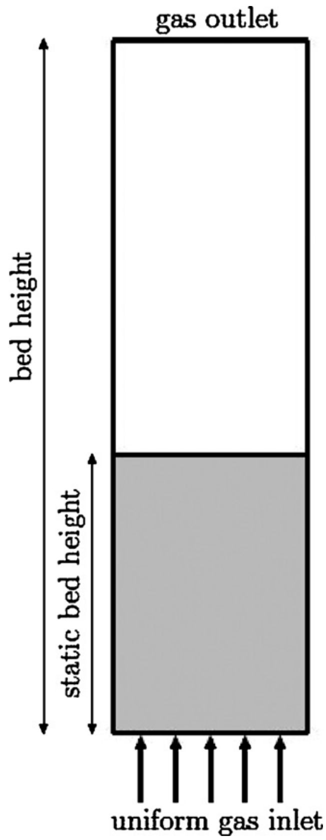


**Fig. 1.** Schematic drawing of 2D bed (Taghipour, Ellis, & Wong, 2005).

influenced by wall effects. As the particle-phase is modeled as a fluid in the Eulerian method, it is necessary to introduce a model for particle–particle interactions. These models usually appear either as additional source term, solids pressure, in the momentum equations or they are included in the viscosity. Two main approaches exist. Firstly, the powder modulus, or particle normal force model, which only affects the solid pressure, and secondly, kinetic theory granular flow which is analogous to the kinetic theory of dense gases.

The kinetic theory of granular flow model gives values for the shear and bulk viscosity of the solid-phase, as well as for solids pressure. This approach is more complicated but physically a complete model for particle–particle interactions. It is based on a suggestion by Ogawa, Unemura, and Oshima (1980), that the mechanical energy is first transformed into random particle motion, instead of dissipating directly to heat. They also derived a conservation equation to describe the transport of the small scale random particle motion. In kinetic theory the particles are assumed to be smooth and the collisions binary, inelastic and instantaneous (see Gidaspow, 1994). While these are reasonable assumptions at low particle volume fractions, they do not apply in densely packed regions where particles are in extended contact with several particles. In these regions, most of the particle energy is dissipated by the surface friction between sliding particles, instead of in inelastic collisions. Several models were proposed in the literature for the frictional stresses. Johnson and Jackson (1987) derived equations for stresses and dissipation of granular temperature caused by particle–wall interactions. They added the frictional and collisional stresses on the wall to the bulk stress of the particle-phase in the direction of the slip velocity between the particles and the wall. For the granular temperature, they wrote an energy balance between the granular energy flux, the dissipation and the collisional stress in the direction of the slip velocity. The relations they found are described also by Jang and Khonsari (2005) and Passalacqua and Marmo (2009).

Many gas–solid CFD models have been put forth by academic researchers, government laboratories and commercial vendors. These models often differ in terms of both the form of the governing equations and the closure relations, resulting in much confusion in the literature. van Wachem, Schouten, van den Bleek, Krishna, and Sinclair (2001) states that the predictions based on the commonly used governing equations do not differ in terms of macroscopic flow behavior, but differ on a local scale. Flow predictions are not sensitive to the use of different solid stress models or radial distribution functions, as different approaches are very similar in dense flow regimes. However, the application of a different drag model significantly impacts the flow of the solids-phase. Works related to achieving an understanding of the hydrodynamics of gas–solid fluidized beds are first reviewed by Lim, Zhu, and Grace (1995), where special emphasis on high velocity systems and solids mixing was set. The Eulerian approach applied to fluidization was further used by, e.g. Enwald, Peirano, and Almstedt (1996) and Boemer (1997). An overview of the physical models for computational fluid dynamics predictions of multiphase flows was given by van Wachem and Almstedt (2003). They also discussed the capabilities and limitations of multiphase CFD methods.

Numerous studies on the kinetic theory model to predict the momentum exchange due to particle–particle collision have validated the implementation of this approach for modeling fluidized beds. By using the commercial code `CFX-4` Lettieri, Cammarate, Micale, and Yates (2003) performed simulations of gas-fluidized beds. They investigated two different approaches, namely the Eulerian granular model and the particle-bed model. Simulations for the stable fluidization behavior of a Geldart Group A powder (see Geldart, 1973; Gidaspow, 1994) and the formation and development of instabilities in a bubbling and slugging bed of Group B material have been carried out. But, only qualitative comparisons of the results with those obtained using granular kinetic theory were given. In the recent study of Vejahati, Mahinpey, Ellis, and Nikoo (2009) an easy to implement and efficient method for adjustment of Di Felice drag law was proposed. This method is to be more efficient compared to the one proposed by Syamlal, Rogers, and O'Brien (1993). The study also accomplish an extensive assessment of frequently used drag correlations in a large selection of published literature and provide a comprehensive comparison between simulation and experimental results using the variety of the drag models. In the study of Taghipour et al. (2005), both experimental and simulation investigations were applied in a 2D fluidized bed column to enable meaningful comparison of the hydrodynamic results. The numerical simulations were based on commercial CFD software `Fluent 6.0`, with various drag functions applied to calculate momentum exchange coefficients and under consideration of the solid fluctuation energy conservation by the kinetic theory of granular flow. The effects of model parameters such as restitution coefficient were evaluated and compared with experimental data.

It is worthy to mention that, compared to Taghipour et al. (2005), our simulations were carried out with a more recent version of `Fluent`, and thus the obtained results matched much better with numerical results of `MFIX`. Concerning `OpenFOAM`, our study shows that the Eulerian–Eulerian module is not yet fully developed. Even if Londono et al. (2007) have tried to benchmark the `OpenFOAM` module based only on global values, our more precise study shows that this code needs improvements. Nevertheless, this module is in further development by Passalacqua and Fox (2011).

The paper is organized as follows: in Section 2 the benchmark problem and the solution procedure are summed up. Global characterizations of the fluidization process, including pressure drop and bed expansion ratio, are discussed in Section 3. In Section 4 instantaneous and statistically averaged flow fields simulated with

MFIX and Fluent are compared among each other. Conclusions are summed up in Section 5.

## 2. Benchmark problem – 2D fluidized bed

This work focuses on the simulation of a two-dimensional fluidized bed column from Taghipour et al. (2005). A schematic drawing of the 2D bed is given in Fig. 1. CFD simulations were conducted using three codes, namely, the open-source solver MFIX (Benyahia, Syamlal, & O'Brien, 2006; Syamlal, O'Brien, Benyahia, Gel, & Pannala, 2008), the commercial solver Fluent version 6.3 (Fluent Inc., 2006) and the open-source code OpenFOAM (Peltola, 2009; Rusche, 2002; Silva & Lage, 2007; Weller, Tabor, Jasak, & Fureby, 1998). Two solvers included in OpenFOAM were used, the twoPhaseEulerFoam module from version 1.6 and twoPhaseEulerPimpleFoam from the most recent version 2.0, where the Pimple method refers to a merged PISO/Simple approach for solving the unsteady Navier–Stokes equations. The simulation model parameters are summarized in Table 1. In this study the bed hydrodynamics and bubble behavior were analyzed for two drag functions including the model of Gidaspow (1994) and that of Syamlal et al. (1993). The Syamlal–O'Brien drag model is derived for a single spherical particle in a fluid, and modified with a relative velocity correlation, which is the terminal settling velocity of a particle in a system divided by the terminal settling velocity of a single sphere, (Ramesh & Raajenthiren, 2010). The Gidaspow drag model is a combination of the Wen-Yu drag model and the Ergun equation. The first one uses a correlation from the experimental data, which is valid when the internal forces are negligible and that the viscous forces dominate the flow behavior, while the second equation is derived for a dense bed and relates the drag to the pressure drop through porous media. For closure of the solids stress terms the kinetic theory of granular flow was used and the algebraic model was principally chosen. Simulations where the transport equation approach was inserted show not significantly differences compared to those where the algebraic model was inserted, but the computational costs are according to van Wachem et al. (2001) much higher. The simulation results were compared against experimental and numerical data of Londono et al. (2007) and Taghipour et al. (2005).

The experimental geometrical dimensions of the fluidization bed were the same as those of Taghipour et al. (2005), namely 1 m height, 0.28 m width and 0.025 m depth. The 2D computational domain was discretized by 11,200 rectangular cells, corresponding to a grid width of $\Delta x = 5$ mm. The time step was $10^{-5}$ s and all simulations were carried out for 12 s real time. Simulations were also carried out on a finer mesh with $\Delta x = 2.5$ mm, but the reached inflow velocity at which simulations are possible is not higher and the computational cost were very high. The bottom of the fluidized bed was made impenetrable for the solid-phase by setting the solid-phase axial velocity to zero and a Dirichlet boundary condition was employed with uniform gas inlet velocity. At the freeboard top the pressure was fixed to a reference value corresponding to a fully developed flow. The left and right walls of the fluidized bed were treated as non-slip and impenetrable walls for both phases. All three used CFD codes give the opportunity to set the Johnson and Jackson partial slip boundary condition for the particle phase at the walls (Johnson & Jackson, 1987). Numerical data analysis were performed to identify the steady state pressure drop $\Delta p$ and bed expansion ratio $H/H_0$, at different superficial gas velocities. According to Taghipour et al. (2005) at the experimentally determined minimum fluidization velocity, $U_{mf} = 0.065$ m/s, the overall pressure drop, bed expansion ratio and voidage, i.e. the gas-phase volume fraction, were 4400 Pa, 1.1 and 0.5, respectively. For the CFD simulations various superficial gas velocities up to 0.5 m/s corresponding to $7.7U_{mf}$ were examined.

**Table 1**
Simulation model parameters of the 2D fluidization bed from Taghipour et al. (2005).

| | | |
|---|---|---|
| Bed width | | 0.28 m |
| Bed height | | 1 m |
| Static bed height | $H_0$ | 0.4 m |
| Grid interval spacing | $\Delta x$ | 0.005 m |
| Particle density | $\rho_s$ | 2500 kg/m$^3$ |
| Gas density | $\rho_g$ | 1.225 kg/m$^3$ |
| Gas kinematic viscosity | $\nu_g$ | $1.485 \times 10^{-5}$ m$^2$/s |
| Mean particle diameter | $d_s$ | 275 μm |
| Initial solids packing | $\alpha_s$ | 0.6 |
| Restitution coefficient | $e$ | 0.9 |
| Superficial gas velocity | $u$ | 0.025–0.51m/s |
| Min. fluidization velocity | $U_{mf}$ | 0.065 m/s |

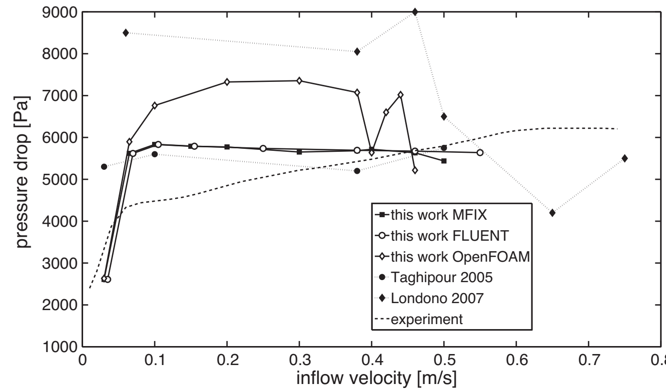


**Fig. 2.** Comparison of MFIX, Fluent and OpenFOAM simulated pressure drop values with existing numerical data of Taghipour et al. (2005), and Londono, Londono, Molina, and Chejne (2007) and experimental data from Taghipour et al. (2005) for the Gidaspow drag model.

## 3. Global characterization of the fluidization process

Due to the transient manner in which bubbles split and coalesce, pressure drop fluctuations are expected in the fluidized bed. In order to eliminate the large temporal fluctuation of pressure drop in the early seconds of the simulation, the time-average of pressure drop for comparing simulation results were taken after statistical steady state was established. Numerical simulations with the 3 CFD codes confirm the statement from Taghipour et al. (2005) that 3 s of simulation time is adequate to reach statistical steady state behavior for all drag function models. Therefore, time-averaging was carried out over a range of 3–12 s of realtime simulation. Figs. 2 and 3 show the pressure drop variation inside the bed as the

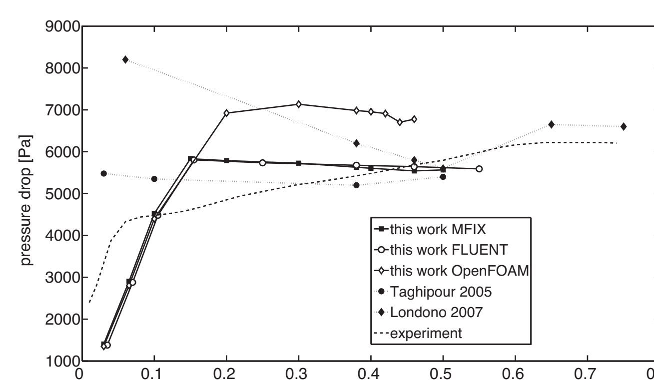


**Fig. 3.** Comparison of MFIX, Fluent and OpenFOAM simulated pressure drop values with existing numerical data of Taghipour et al. (2005), and Londono et al. (2007) and experimental data from Taghipour et al. (2005) for the Syamlal–O'Brien drag model.

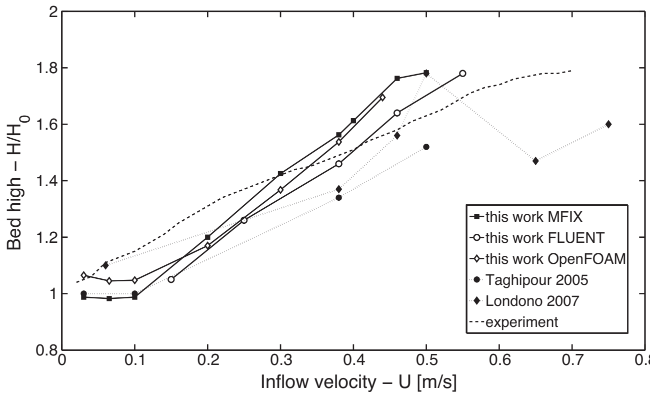


**Fig. 4.** Comparison of `OpenFOAM`, `MFIX` and `Fluent` simulated bed expansion ratio with existing data for Syamlal–O'Brien drag model.

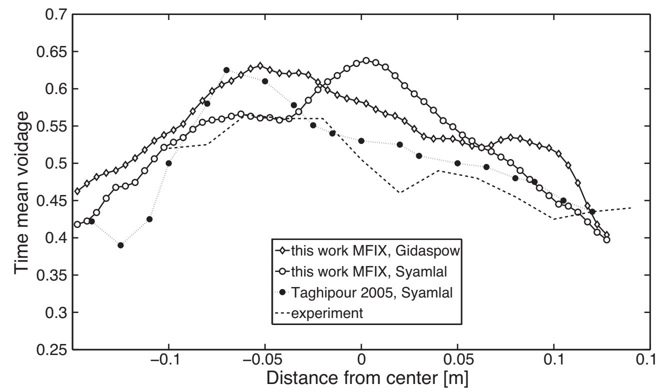


**Fig. 5.** Time-average local voidage profiles for $U_{in}$ = 0.38 m/s at $z$ = 0.2 m. Time averaging over 3–12 s.

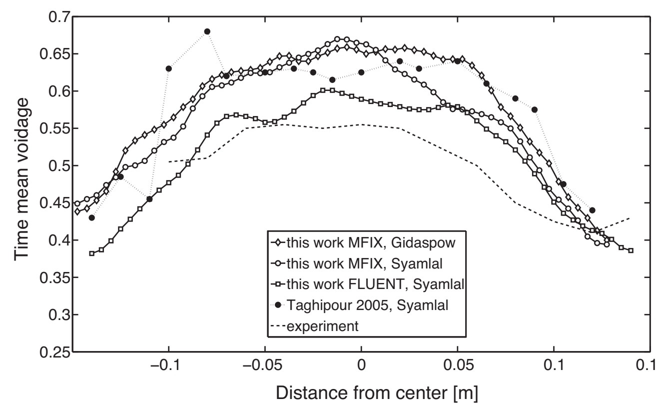


**Fig. 6.** Time-average local voidage profiles for $U_{in}$ = 0.46 m/s at $z$ = 0.2 m. Time averaging over 3–12 s.

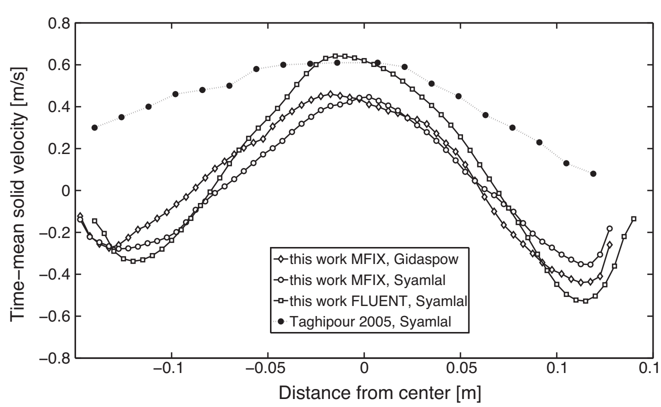


**Fig. 7.** Time-average solid velocity profiles for $U_{in}$ = 0.46 m/s at $z$ = 0.2 m. Time averaging over 3–12 s.

superficial gas velocity increases using Gidaspow and respectively Syamlal–O'Brien drag model. Both figures describe typical fluidized bed behavior. When the inflow gas velocity reaches the minimum fluidization velocity $U_{mf}$, the bed pressure drop starts to increase continuously until it reaches a maximum pressure drop value. This pressure drop value remains nearby constant showing a relative plateau trend with increasing gas velocity for both drag models, which is in good agreement with both theoretical and experimental predictions. Our simulations with `MFIX` and `Fluent` give very similar pressure drop values, which are comparable to the numerical and experimental results of Taghipour et al. (2005). Moreover, at low but higher than $U_{mf}$ inflow gas velocities, the pressure drop values given by all three codes show the same ascendent behavior like the experimental data but contrary to the numerical results from Taghipour et al. (2005). Especially for Syamlal–O'Brien drag model the numerical pressure drop from Taghipour et al. (2005) has much higher and descendent values. By further increasing of the inflow velocity the established plateau of our `MFIX` and `Fluent` results coincide and are situated slightly higher than the numerical results of Taghipour et al. (2005) for both drag models. For the highest inflow velocities reached in our simulations, very similar values to the numerical and experimental data of Taghipour et al. (2005) were yielded with the two above mentioned codes. In the plateau region our `OpenFOAM` simulations as well as that of Londono et al. (2007) differ essentially from the other curves. Nevertheless, for the highest inflow velocities also `OpenFOAM` results of Gidaspow's drag model simulations matched quite well to the pressure drop values obtained with the other codes. The bed expansion ratio was calculated from the pressure drop along a vertical line in the middle of the bed. The time-average bed expansion ratio is plotted in Fig. 4 for various gas inflow velocities. Here, simulations using Syamlal–O'Brien drag function are compared with existing numerical and experimental data. A consistent increase in bed expansion with gas velocity is demonstrated by using all three CFD codes. At lower inflow velocities the bed expansion is quite constant for our `MFIX` and `OpenFOAM` simulations and at higher inflow velocity values all three codes predicted the relative bed high reasonably well.

Further, the numerical time-average cross-sectional voidage profiles at $z$ = 0.2 m are compared to existing numerical and experimental data in Figs. 5 and 6 for inflow gas velocity $U_{in}$ = 0.38 and 0.46 m/s, respectively. Like in Taghipour et al. (2005) also in our simulation results one can also observe the increased symmetry of the voidage profile for $U_{in}$ = 0.46 m/s compared to those corresponding to $U_{in}$ = 0.38 m/s. The slight asymmetry in the voidage profile for $U_{in}$ = 0.38 m/s may result from the development of certain flow patterns and bubbles in the bed. The maximal mean voidage values obtained with `MFIX` for both drag models are comparable to that of Taghipour et al. (2005).

Comparisons of the solid velocity profiles at $U_{in}$ = 0.46 m/s indicate also a very good agreement. As shown in Fig. 7, the numerical simulations with `MFIX` and `Fluent` yield parabolical profiles in the bed interior and a downward flow near the side walls.

## 4. Flow fields visualization

To deliver a more precisely insight into the fluidization phenomena hydrodynamics, instantaneous and time averaged gas and solid flow fields obtained with `MFIX` and `Fluent` are put side by

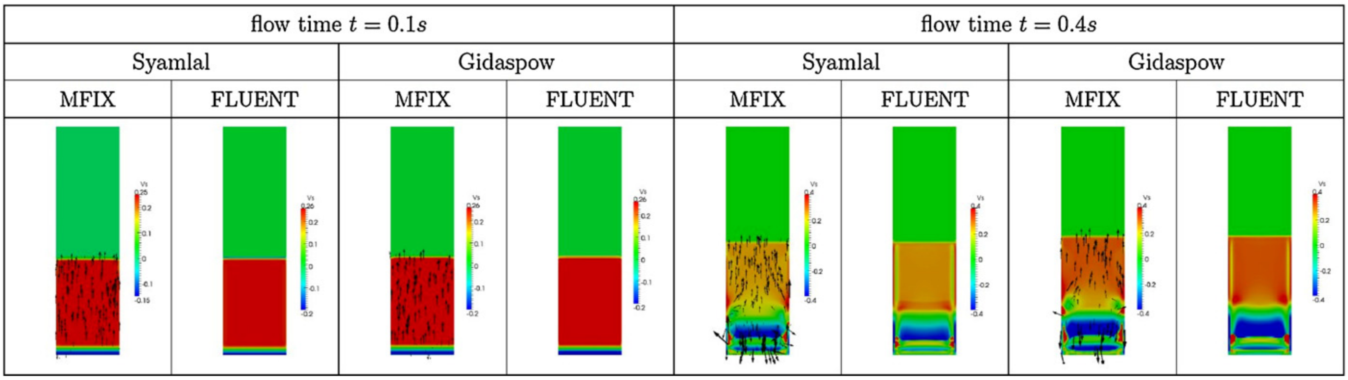


**Fig. 8.** Snapshots of solids velocity field for inflow velocity $U_{in}$ = 0.38 m/s. Axial velocity component and velocity vectors.

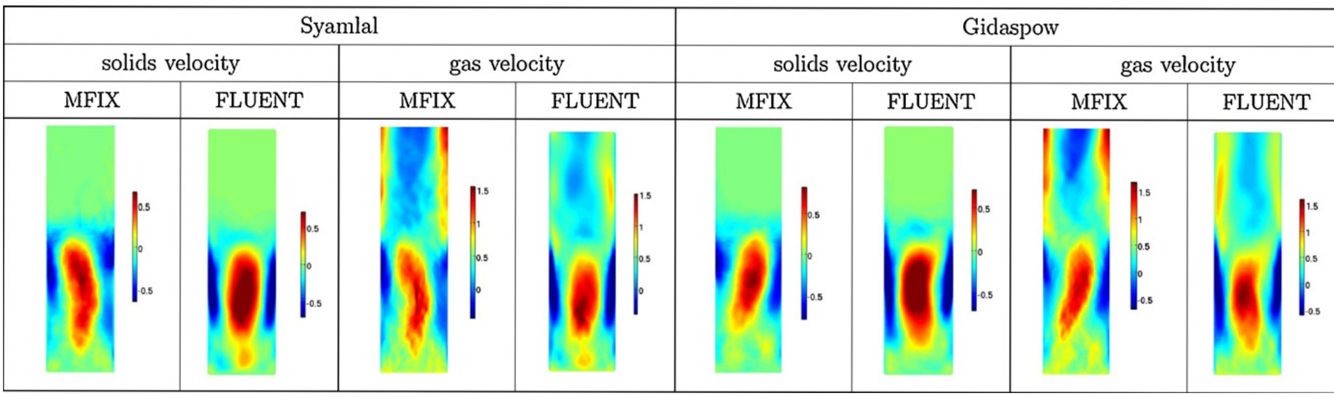


**Fig. 9.** Syamlal–O'Brien and Gidaspow drag models, time averaged solids and gas axial velocity component over a range of 3–9 s of realtime simulation for inflow velocity $U_{in}$ = 0.38 m/s.

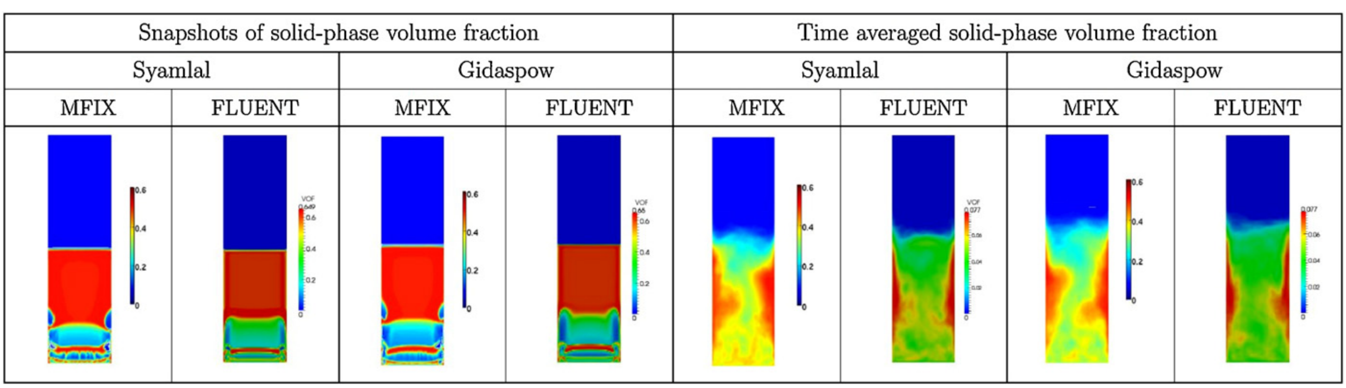


**Fig. 10.** Snapshots of solid-phase volume fraction at the flow time $t$ = 0.4 s and time averaged solid-phase volume fraction for inflow velocity $U_{in}$ = 0.38 m/s.

side. Snapshots of solids velocity axial component at simulated flow times 0.1 s and 0.4 s are given in Fig. 8. A similar bubble formation and development way can be observed at simulation beginning for both codes for Syamlal–O'Brien as well as for Gidaspow's drag function. Also, the time-averaged solids and gas velocity fields over a range of 3–9 s of realtime simulation, show in Fig. 9 a very good agreement between `MFIX` and `Fluent` numerical results. The time-averaged solid velocity fields, offer an upward flow in the bed interior and a downward flow near the side walls. By comparing the simulated velocity fields corresponding to Syamlal–O'Brien drag model with those corresponding to Gidaspow's one of the same numerical code, no significant pattern differences exist.

Fig. 10 shows the solids volume fraction profile for inflow velocity $U_{in}$ = 0.38 m/s at 0.4 s simulation time and the time-averaged solids volume fraction over a range of 3–9 s. Numerical results of `MFIX` and `Fluent` are quite similar for both drag models.

## 5. Conclusion

The influence of most widely used drag functions, including the Syamlal et al. (1993) and Gidaspow (1994) models on CFD simulation of a 2D fluidized bed benchmark of Taghipour et al. (2005) was studied. Three CFD software packages were used, namely, `MFIX`, `Fluent` and `OpenFOAM`, and the obtained results were compared among themselves for gas inflow velocities up to 0.5 m/s. Both drag models showed an acceptable qualitative agreement with existing numerical and experimental data. Global values, like pressure drop and bed expansion ratio, are in good agreement for all three numerical codes. Especially, the pressure drop values provided by MFIX conform exactly with those of Fluent. The shape of the time-average local voidage profiles is similarly. Snapshots of the flow fields show a very good agreement between the MFIX and Fluent simulations, but do not conform with those of OpenFOAM. Thus, the fluidized bed benchmark simulations presented in this paper show that the development of the open-source MFIX code and also of the commercial product Fluent is technically mature to predict well fluidization phenomena based on the Eulerian–Eulerian method. Further efforts are required to model the benchmark problem with OpenFOAM and to study the influence of other parameters such as gas distributors or geometry variations like fluidized bed containing horizontal tubes (Asegehegn & Krautz, 2009). Comparison of 2D and 3D modeling of fluidized bed reactors and effect of particle size distribution, which has been underestimated using the mean particle diameter, are further tasks.

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