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MULTIPHASE CFD FOR GAS-PARTICLE FLOWS: BEYOND THE TWO-FLUID MODEL

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ABSTRACT

The accurate prediction of dilute gas-particle flows using Euler-Euler models is challenging because particle-particle collisions are usually not dominate in such flows. In other words, in dilute flows the particle Knudsen number is not small enough to justify a Chapman-Enskog expansion about the collision-dominated equilibrium limit. Moreover, due to the fluid drag and inelastic collisions, the granular temperature in gas-particle flows is often small compared to the mean particle kinetic energy, implying that the particle-phase Mach number can be very large. In analogy to rarefied gas flows, it is thus not surprising that two-fluid models fail for gas-particle flows with moderate Knudsen and/or Mach numbers.

In this work, a third-order quadrature-based moment method, valid for arbitrary Knudsen number, coupled with a fluid solver has been applied to simulate dilute gas-particle flow in a vertical channel with particle-phase volume fractions between 0.0001 and 0.01. In order to isolate the instabilities that arise due to fluid-particle coupling, a fluid mass flow rate that ensures that turbulence would not develop in a single phase flow (Re = 1380) is employed. Results are compared with the predictions of a two-fluid model with standard kinetic theory based closures for the particle phase. The effect of the particle-phase volume fraction on flow instabilities leading to particle segregation is investigated, and differences with respect to the two-fluid model predictions are examined.

NOMENCLATURE

C	collision integral
e_p	particle-particle restitution coefficient
e_w	particle-wall restitution coefficient
f	velocity distribution function
f^*	equilibrium velocity distribution function
$\mathbf{F}$	force acting on each particle
$\mathbf{g}$	gravitational acceleration vector
Kn	particle phase Knudsen number
m_p	particle mass
M_{ijk}	moment of order $i+j+k$
M^i	moment of order i
$\mathbf{M}_{gs}$	momentum exchange term
p	pressure
Re	fluid-phase Reynolds number
t	time
$\mathbf{U}_g$	fluid-phase mean velocity
$\mathbf{v}$	particle velocity
α_g	fluid-phase volume fraction
α_s	fluid-phase volume fraction
ρ_g	fluid-phase density
ρ_s	fluid-phase density
μ_g	fluid-phase dynamic viscosity
τ_c	collision time
$\boldsymbol{\tau}_g$	fluid-phase stress tensor

INTRODUCTION

Gas-particle flows represent an important class of multiphase flows that occur in many in fields of engineering. For example, chemical processes utilizing fluidized beds and risers are widely used in a variety of processes. In aerospace engineering, gas-particle flows are of great interest in helicopter design due to brownout phenomenon. Likewise, in other scientific fields such as medicine (inhalers design), and vulcanology (dispersion of eruptive material in the atmosphere) gas-particle flows play an important role.

The most exact treatment of gas-particle flows would completely resolve the flow field around each particle as well as all of the turbulent structures in the gas phase. The computational cost of such an approach limits its applicability to simple canonical flows. At the next level of approximation, gas-particle flows can be described by solving the fluid-phase continuity and momentum equations, modified to account for interactions with the dispersed phase. These interactions include the volume-displacement effect (volume fraction) and momentum exchange. The particle phase may be described with a variety of methodologies, all based on the analogy between the dispersed phase and a granular gas. For example, the discrete particle method (DPM) (Hoomans et al., 1996) accounts for individual particle-particle collisions and uses a mean-field drag model to describe fluid-particle momentum exchange. In theory, a granular gas is governed by a kinetic equation for the particle velocity number density function $f(t,\mathbf{x},\mathbf{v})$. The particle-phase kinetic equation has terms for transport, body forces, fluid drag, and collisions, and is valid for arbitrary values of the particle-phase Knudsen and Stokes numbers. However, the exact collision term in the kinetic equation is not closed (e.g., for hard-sphere binary collisions) and a closure must be introduced to replace the two-particle number density function by a function of $f(t,\mathbf{x},\mathbf{v})$ (e.g., the Boltzmann collision integral).

Even after closure, the direct solution of the particle-phase kinetic equation is extremely expensive and one usually

resorts to approximate solutions. For example, in the small Knudsen number limit, a Chapman-Enskog expansion can be used to derive a 'hydrodynamic' description of the particle phase. This is the approach used to develop the two-fluid model (Gidaspow, 1994) for gas-solid flows and, hence, one cannot expect the two-fluid model to be valid when finite-Knudsen effects are important.

Approximate solutions to the kinetic equation can also be found using Lagrangian methods based on discrete simulation Monte Carlo (DSMC) (Bird, 1994). In this approach, each particle trajectory is tracked individually and collisions are described in a statistical manner that is consistent with the *closed* collision term. (In other words, DSMC is less exact than DPM due to the treatment of collisions.) If sufficiently large numbers of particles are tracked in order to suppress statistical errors, the DSMC approach can yield very accurate solutions to the kinetic equation. Nevertheless, for practical systems it is limited to flows with relatively low particle-phase volume fractions, due to its computational cost. In general, the cost of DSMC (and DPM) increases with the particle concentration because the number of particles to be tracked increases and because of the increasing number of collisions that must be detected.

Lagrangian multiphase particle-in cell (MP-PIC) methods (Andrew and O'Rourke, 1996; Patankar and Joseph, 2001; Snider, 2001) can also be used to approximate gas-particle flows. However, this approach does not accurately describe the collision term in the kinetic equation. Instead, particles are grouped into 'parcels' to reduce the computational cost in the dense limit where collisions are dominant. In some implementations, to further reduce the computational cost, only an isotropic stress tensor is added to the MP-PIC formulation to enforce the maximum particle packing limit (Snider, 2001). This approximation limits the capabilities of the approach to properly predict particle segregation in polydisperse flows. More generally, unlike DSMC, the MP-PIC approach does not attempt to accurately reproduce the terms in the underlying kinetic equation by carefully controlling the statistical errors due to finite sample sizes. As shown by Passalacqua et al. (2009), statistical errors in Lagrangian methods strongly affect the instabilities observed in fully coupled gas-particle flow solvers.

Eulerian approaches to approximating the kinetic equation consider a set of moments of the number density function, and track their evolution in space and time. This class of methods goes under the name of the method of moments, and various flavours can be applied to the simulation of gas-particle flows. One popular Eulerian approach is represented by two-fluid models, where only the lowest-order moments (number density, mean momentum and granular temperature) of the particle velocity distribution are considered. In two-fluid models, the fluid-dynamic properties of the granular phase are evaluated using moment closures obtained from the kinetic theory of granular flows under the hypothesis of near-equilibrium, collision-dominated flow (Gidaspow, 1994; Enwald, 1996). This limit corresponds to a particle Knudsen number near zero, which prevents the two-fluid model from properly predicting the behaviour of gas-particle flows in which rarefaction effects play an important role.

Recently novel Eulerian approaches have been investigated to work around the shortcomings of the two-fluid model. For example, Sakiz and Simonin (1998) adopted the Grad (1949) approach to study non-equilibrium phenomena in very dilute riser flows (i.e., with one-way coupling). Desjardin et al. (2008) used a quadrature-based moment method to show the limitations of the two-fluid model in predicting *particle trajectory crossing*, which leads to inconsistent predictions by the hydrodynamic model for all the velocity moments for non-zero Stokes numbers and to the over-prediction of particle segregation. By comparing with Lagrangian simulations of particles in a turbulent flow, Desjardin et al. (2008) showed that intense particle segregation at moderate Knudsen numbers is an artefact (known as a ***delta-shock*** in the mathematical literature) of the mathematical structure of the two-fluid model rather than a true physical phenomenon. In the dilute limit, the particle pressure and particle stress tensor appearing in the two-fluid model are very small since the collision term scales with the square of the particle-phase volume fraction. The mathematical structure of the two-fluid model is then equivalent to the pressure-less gas dynamic equation, the prototypal example for delta-shock formation. Physically, a delta-shock is formed when faster moving particles overtake slower moving particles. In the dilute limit, the faster particles simply pass by the slower particles, a phenomenon that is accurately captured by Lagrangian methods. In the two-fluid model (and any other model based on Chapman-Enskog-like expansions), the local particle velocity is ***single-valued***, causing particles to artificially collide when the fast particles try to pass the slow ones. The method developed by Desjardin et al. (2008) overcomes this fundamental shortcoming of the two-fluid model by allowing the local particle velocity to be ***multi-valued***.

In a coupled gas-particle flow, the inability to capture particle trajectory crossing has profound effects on the entire simulation. First, particles artificially cluster when they should not, leading to dense particle zones in an otherwise dilute flow. These dense regions then change the evolution of the gas-phase flow through the coupling terms, leading to a completely different overall flow structure. Moreover, because by definition a delta-shock is concentrated on a lower-dimensional manifold in three-dimensional space, it is impossible to obtain a grid-independent solution for the two-fluid model in the dilute limit (i.e., whenever the particle-pressure term is too weak to eliminate delta-shocks). In practice, grid refinement will cause the gas-particle flow to become completely segregated into dense structures separated by particle-free zones. Such intense segregation is not observed in Lagrangian simulation or experiments (He et al. 2009) of dilute gas-particle flows.

Another significant shortcoming of the two-fluid model is the treatment of particle-wall collisions under dilute conditions. By definition, a specular collision with a wall leads to a bi-modal velocity distribution function with one mode corresponding to the incoming velocity, and the other to the outgoing velocity. Due to insufficient particle-particle collisions in the region next to the wall, in dilute gas-particle flows the resulting 'Knudsen layers' can extend far away from the walls. In terms of the moments of the velocity distribution function, specular collisions result in an *increase* in the granular temperature at the

wall, causing particles to move away from the wall. In contrast, in the two-fluid model the granular temperature near the wall found using specular collisions is small, resulting in an artificial clustering of particles in the low-temperature zone next to the wall.

In order to better capture the physics of dilute gas-particle flows, Fox (2008) developed a third-order quadrature-based moment method (QMOM) that has recently been implemented into the CFD code MFIX (Syamlal, 1998) by Passalacqua et al. (2009). These authors have validated the MFIX-QMOM approach against Lagrangian and two-fluid simulations and showed that the values of the particle-phase Knudsen and Mach numbers in moderately dilute gas-particle flows are well above the range of validity of hydrodynamic models with partial-slip boundary conditions. In this work the MFIX-QMOM code is applied to simulate dilute gas-particle flows in a vertical channel with particle-phase volume fractions in the range [0.01, 0.0001]. As in our previous work, the fluid-phase mass flow rate is chosen such that the fluid Reynolds number is below the transition to turbulence for a single-phase flow. Whenever possible, results are compared with the predictions of the two-fluid model in MFIX.

MODEL DESCRIPTION

Fluid-phase equations

In the MFIX-QMOM code, the fluid-phase equations are the conventional two-fluid equations for the continuous phase:

$$\frac{\partial}{\partial t}\left(\alpha_g \rho_g\right) + \nabla \cdot \left(\alpha_g \rho_g \mathbf{U}_g\right) = 0$$

$$\frac{\partial}{\partial t}\left(\alpha_g \rho_g \mathbf{U}_g\right) + \nabla \cdot \left(\alpha_g \rho_g \mathbf{U}_g \mathbf{U}_g\right) = \nabla \cdot \boldsymbol{\tau}_g + \alpha_g \rho_g \mathbf{g} + \mathbf{M}_{gs}$$

where $\mathbf{M}_{gs}$ is the momentum transfer term. Details on how the fluid-phase equations are coupled to the particle-phase description can be found in Passalacqua et al. (2009).

Particle-phase moment transport equations

The moment transport equations used in the MFIX-QMOM code are obtained by applying the definition of velocity moments of the particle velocity number density function:

$$m^{\gamma} = \int \mathbf{v}^{\gamma} f(t, \mathbf{x}, \mathbf{v}) d\mathbf{v},$$

where γ is the order of the moment, to both sides of the kinetic equation:

$$\partial_t f + \mathbf{v} \cdot \partial_{\mathbf{x}} f + \partial_{\mathbf{v}} \left(f \frac{\mathbf{F}}{\mathrm{m_p}} \right) = C$$

where $\mathbf{v}$ is the particle velocity, $\mathbf{F}$ the force acting on each particle, m_p the particle mass and C is the rate of change of f due to collisions. The drag term is modelled according to Schiller and Neumann (1935), with the correction proposed by Wen and Yu (1966) to account for the effect of the gas-phase volume fraction:

$$\mathbf{F} = \frac{3 \mathrm{m_p} \rho_g}{4 \mathrm{d_p} \rho_p} C_d \left| \mathbf{U}_g - \mathbf{v} \right| \left(\mathbf{U}_g - \mathbf{v} \right)$$

$$C_d = \frac{24}{\alpha_g \mathrm{Re_p}} \left(1 + 0.15 \left(\alpha_g \mathrm{Re_p} \right)^{0.687} \right) \alpha_g^{-2.65}$$

The collision term is closed using the linearized model proposed by Bahatnagar et al. (1954):

$$\mathrm{C} = \frac{1}{\tau_c} \left(f^* - f \right),$$

where the collision time τ_c has been modified to include the radial distribution function, which makes the collision frequency increase for increasing particle-phase volume fraction.

If the set of moments considered to approximate the solution of the kinetic equation is truncated at third order (Fox, 2008), the resulting twenty (one equation for M^0 (continuity), three for $\mathbf{M^1}$ (mean momentum), six for $\mathbf{M^2}$ (particle stress tensor) and ten for $\mathbf{M^3}$) moment transport equations are given by

$$\frac{\partial M^0}{\partial t} + \frac{\partial M_i^1}{\partial x_i} = 0$$

$$\frac{\partial M_i^1}{\partial t} + \frac{\partial M_{ij}^2}{\partial x_j} = g_i M^0 + D_i^1$$

$$\frac{\partial M_{ij}^2}{\partial t} + \frac{\partial M_{ijk}^3}{\partial x_k} = g_i M_j^1 + g_j M_i^1 + C_{ij}^2 + D_{ij}^2$$

$$\frac{\partial M_{ijk}^3}{\partial t} + \frac{\partial M_{ijkl}^4}{\partial x_l} = g_i M_{jk}^2 + g_j M_{ik}^2 + g_k M_{ij}^2 + C_{ijk}^3 + D_{ijk}^3$$

where the spatial derivatives represent the moment spatial fluxes, $\mathbf{g}$ is gravitational acceleration, D are the source terms due to the drag force, and C are the source terms due to collisions. The moment spatial fluxes are computed in terms of the quadrature weights and abscissas, relying on their kinetic definition (Desjardin et al., 2008). Details on the derivation of the quadrature-based closures are reported in Fox (2008), their implementation can be found in Passalacqua et al. (2009), and is not repeated here.

The two-fluid model simulations were performed using the kinetic theory closures obtained by Gidaspow (1994) and implemented in MFIX (Syamlal, 1998). In the MFIX code, the complete transport equation for the granular energy is solved, neglecting only the term due to the fluid-particle velocity correlation.

DESCRIPTION OF THE PROBLEM

A gas-particle flow in a two-dimensional vertical channel (0.1 x 1 m) with monodisperse particles was considered. The mass flow rate of the fluid-phase (ρ_g = 1.2 kg/m^3) was fixed so that the fluid-phase Reynolds number is 1380, well below the transition to turbulence in a single-phase flow. This choice was made to remove the direct effect of the fluid turbulence on the formation of segregated structures from the system. The desired fluid-phase Reynolds number was obtained by setting the viscosity of the fluid phase to μ_g = 1.74 x 10^{-4} Pa s.

For the particle phase, a range of volume fractions between 0.0001 and 0.01 was considered, with a particle density of 1500 kg/m^3. The particle diameter was set to 252 μm, and the restitution coefficients for both particle-particle and particle-wall collisions were set to $e_p = e_w = 1$, which corresponds to perfectly elastic collisions.

Wall boundary conditions were set to be specularly reflective. This condition is equivalent, in the two-fluid model, to a free-slip condition for the particle phase. No-slip conditions were used at the walls for the fluid phase. Periodic conditions with constant mass flow rates were adopted in the flow direction for both phases. A uniform field for all the properties was used as the initial conditions.

RESULTS

Results of a channel-flow simulation with particle-phase volume fraction of 0.01 obtained with MFIX-QMOM are reported in **Figure 1**, where snapshots of the time evolution of the particle-phase volume fraction are shown. The predictions of the two-fluid model for the same case are show in **Figure 2**. At the beginning of the simulation, the particles, initially distributed uniformly in the channel, are accelerated towards the walls due to the mean fluid velocity gradient, where they are reflected and move towards the centre of the channel. This process leads to the formation of preferential particle-depleted vertical paths for the fluid phase, where it can accelerate. This separation however is unstable, due to the velocity gradient between the zone at low particle concentration and the one at higher particle concentration, as observed in Passalacqua et al. (2009). This leads to chaotic flow behaviour, where particles tend to segregate towards the walls, originating the characteristic core-annular flow, with particles falling along the channel walls, with an oscillating upward flow in the centre.

A similar behaviour is observed in the initial stages of the two-fluid model prediction, where particles are reflected by the walls and give origin to the preferential paths for the fluid phase (**Figure 2**, t = 1.45 s). However, the evolution of the system from this point on proceeds with the formation of two unstable structures on the sides of the flow, which leads to particle segregation. The main difference between the MFIX-QMOM and two-fluid model predictions is, however, the abundance of fine structures at high particle concentration in the two-fluid prediction (i.e., delta-shocks), which are not predicted by the QMOM model. As mentioned earlier, the formation of these structures in two-fluid models can be explained by the fact that when particle trajectory crossing occurs, models tracking only the mean momentum are unable to predict correctly all the velocity moments. In such a situation, hydrodynamic models predict a delta-shock, since they cannot represent a situation where multiple distinct local particle velocities are present. Also, as noted earlier, further grid refinement will exacerbate the segregation in the two-fluid model, whereas the MFIX-QMOM results are essentially grid independent.

Although not as easily distinguished in the snapshots in **Figures 1** and **2** as in flow-field animations, there are also clear differences between the MFIX-QMOM and the two-fluid predictions in the regions near the walls. In the MFIX-QMOM simulations, the falling particles form larger 'blobs' that cover several grids cells away from the wall, while in the two-fluid predictions the falling particles remain much closer to the wall. We believe that these differences can be attributed to the differences in the boundary conditions for the granular temperature.

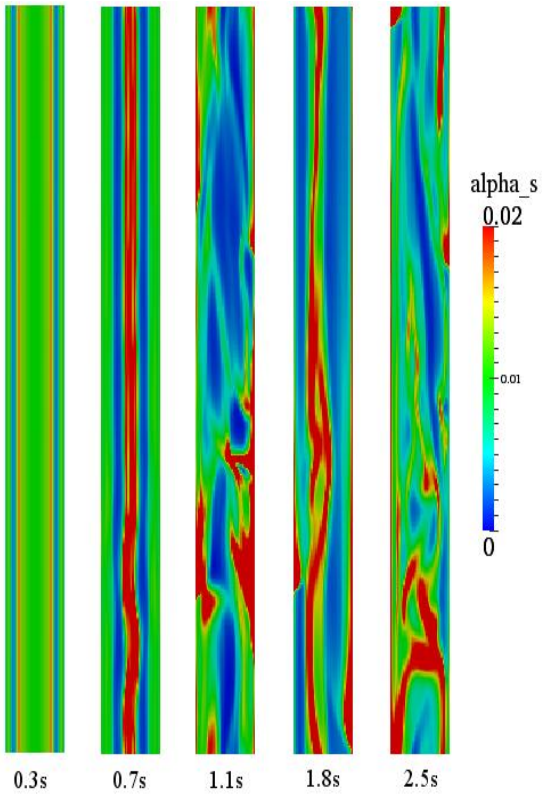

Figure 1: Particle-phase volume-fraction evolution predicted by MFIX-QMOM with an average particle-phase volume fraction of 0.01.

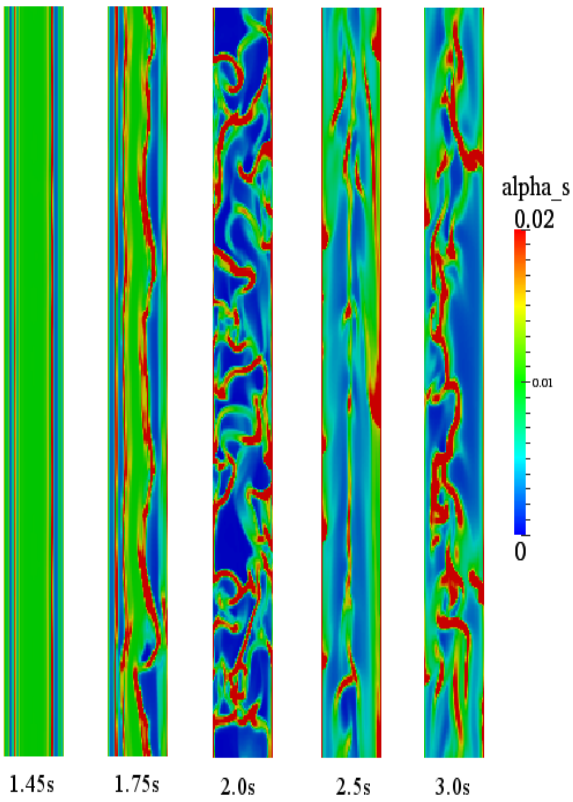

Figure 2: Particle-phase volume-fraction evolution predicted by the two-fluid model with an average particle-phase volume fraction of 0.01.

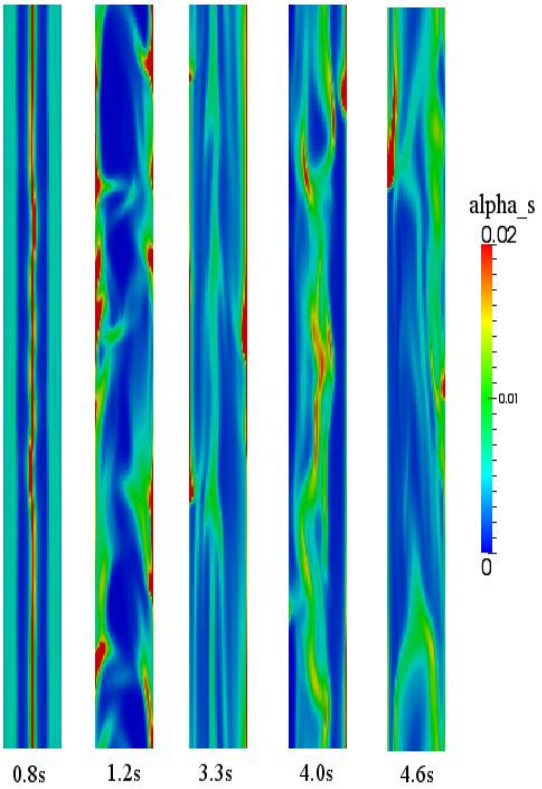

Figure 3: Particle-phase volume-fraction evolution predicted by MFIX-QMOM with an average particle-phase volume fraction of 0.005.

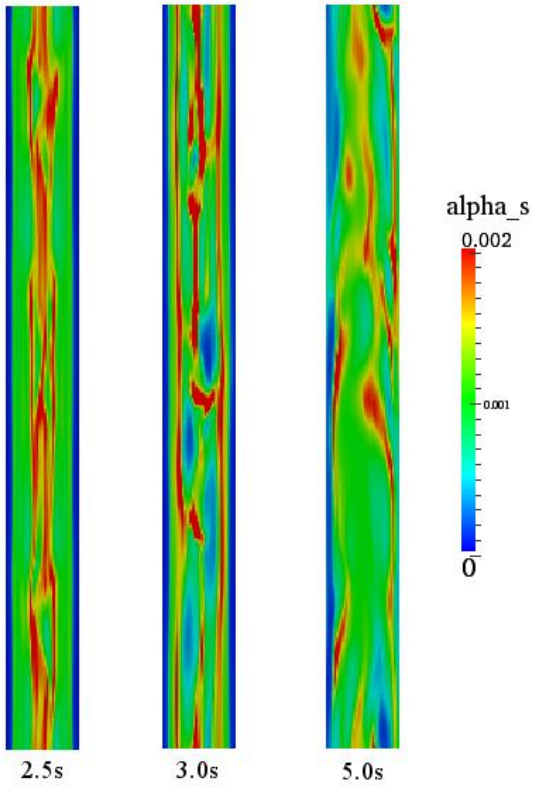

Figure 5: Particle-phase volume-fraction evolution predicted by MFIX-QMOM with an average particle-phase volume fraction of 0.001.

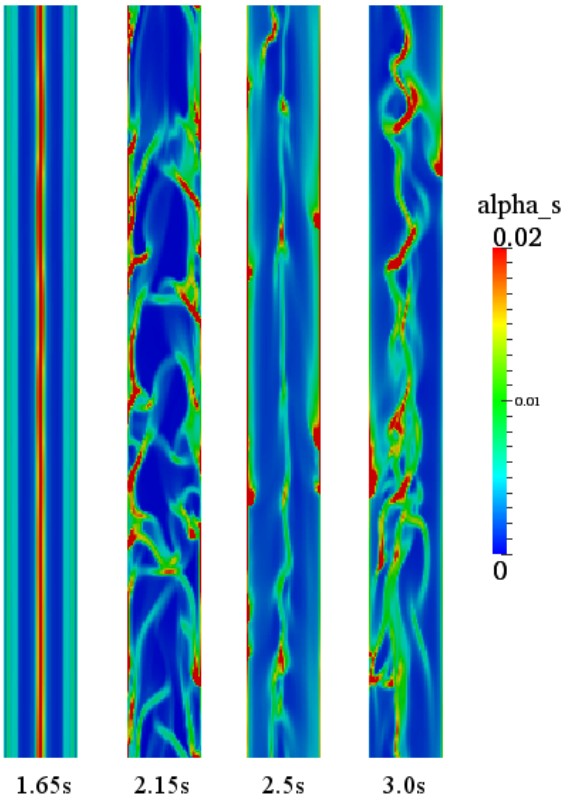

Figure 4: Particle-phase volume-fraction evolution predicted by the two-fluid model with an average particle-phase volume fraction of 0.005.

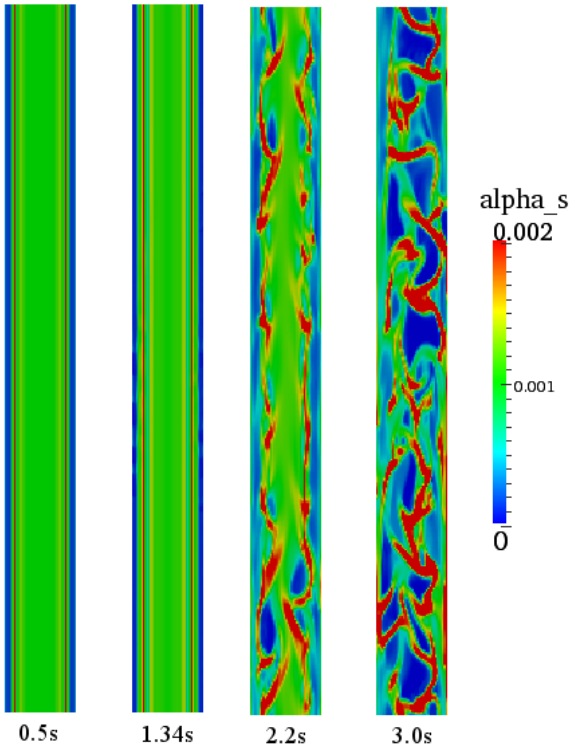

Figure 6: Particle-phase volume-fraction evolution predicted by the two-fluid model with an average particle-phase volume fraction of 0.001.

Similar results were observed in the case of an average particle-phase volume fraction of 0.005, reported in **Figure 3** (MFIX-QMOM) and **Figure 4** (two-fluid model). The agreement between the two predictions is consistent during the initial stages of the simulations. However, the two-fluid model still shows a tendency to predict fine structures at high particle concentration, as observed in the previous case. The effect of the particle concentration on the development of the instability that leads to particle segregation was further investigated by considering two cases with lower mass loading. **Figure 5** shows the evolution of the flow predicted by MFIX-QMOM in the case of an initial mean volume fraction of 0.001, while **Figure 6** reports the prediction of the two-fluid model in the same case. The mechanism that leads to the formation of an unstable flow is similar to that observed in the densest cases. However the transition to an unstable flow, and the consequent particle segregation phenomena, are slower and less evident, since the particle concentration is lower. The two-fluid model predicts a similar behaviour to the one observed in **Figure 2**, with the formation of small structures not observed in the MFIX-QMOM prediction.

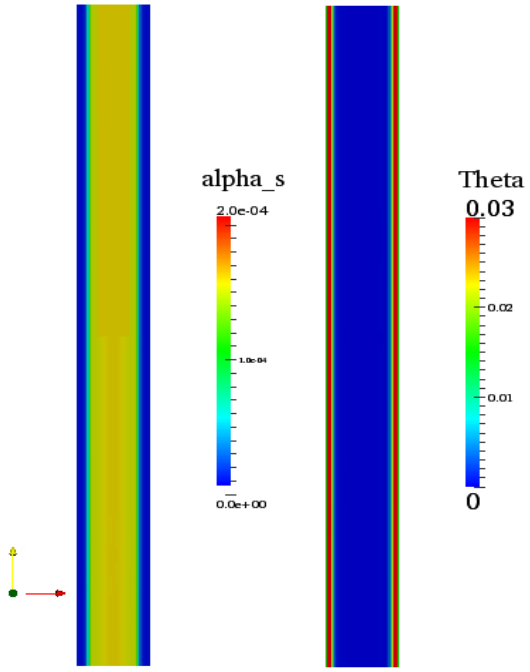

Figure 7: Particle-phase volume fraction and granular temperature at 5 s predicted by MFIX-QMOM with an average particle-phase volume fraction of 0.0001.

An even more dilute case, with an average particle volume fraction of 0.0001 (mass loading 0.13), was also considered. The results of the MFIX-QMOM predictions are reported in **Figure 7**. We did not obtain a convergent solution using the two-fluid model with the required convergence criteria used in the other cases; as a consequence results from two-fluid models are not reported. For this case, after 5 s of simulation time, particles are still distributed almost uniformly across the channel, with the exception of near the walls, since in the wall zone the particle temperature is highest. Although we cannot confirm it directly due to the finite duration of our simulation, it appears that the case shown in **Figure 7** reaches a time-independent state where only gradients in the wall-normal direction are present.

As noted earlier, in the zone next to walls the net particle flux is zero, and, as a consequence the mean particle velocity is zero, but the velocity variance is high due to specular reflections. As observed in Passalacqua et al. (2009), this means that the local particle Mach number of the flow, defined using of the mean particle velocity and the granular temperature (Kogan, 1969), and the local Knudsen number, are large and well outside the range of validity of hydrodynamic models (Kn < 0.1), even with the addition of partial-slip boundary conditions (Bird, 1994; Struchtrup, 2005) like those proposed by Johnson and Jackson (1987). In the cases considered in this work, the Johnson and Jackson boundary conditions degenerate into free-slip conditions, since the walls are assumed to be frictionless. It is worth noting that the Johnson and Jackson boundary conditions imply a zero granular temperature flux at the wall, when perfectly specular conditions are imposed. This implies that the two-fluid models cannot convert the velocity of particles impinging on the wall into granular temperature, even though the velocity component normal to the wall is zero. As a consequence, the maximum in the granular temperature at the walls that is observed in **Figure 7** is not captured by the two-fluid model.

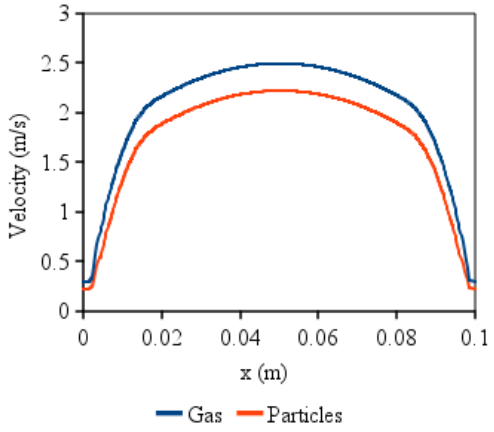

Figure 8: Phase velocities predicted by MFIX-QMOM at 5 sec with an average particle-phase volume fraction of 0.0001.

The vertical velocity profiles for the case in **Figure 7** are reported in **Figure 8**, and show that the flow has the typical profile of a stable channel flow. For this case, the particle mass loading is small enough to not have a destabilizing effect on the fluid phase. However, it is worth noting that the velocity profiles are not perfectly parabolic, due to the presence of the particles and the momentum coupling with the particle phase. Nonetheless, no instabilities develop and both phases attain a steady state.

CONCLUSIONS

A set of simulations of particle-laden channel flow with finite Stokes number particles at different average

concentrations were performed. A third-order quadrature-based moment method was used to describe the particle phase by approximating its kinetic equation.

The formation of small local structures at higher particle concentration in the two-fluid model was discussed. It has been shown that, at the same operating conditions, local intense segregation phenomena are not predicted by a higher-order approximation of the kinetic equation that allows multiple local velocities. It was also shown how the particle-phase average volume fraction influences the development of flow instabilities, which lead to particle segregation. In a sufficiently dilute case, these instabilities did not appear in the MFIX-QMOM simulations.

The relative computational cost of MFIX-QMOM with respect to the two-fluid model in MFIX is in the range of 1.5–1.9. The longest simulation was the one with the highest particle-phase volume fraction, which required 25.37 hours with the two-fluid model and 48.2 hours with MFIX-QMOM on a single core of an Intel Xeon CPU at 3.0GHz. It is worth noting that the hyperbolic nature of the QMOM model should make the MFIX-QMOM code highly scalable. In the dilute limit, the time step is limited only by the CFL number and the kinetic-based fluxes are stable for relatively large CFL number (e.g., CFL=1 for the first-order scheme).

Work is in progress to extend the MFIX-QMOM code discussed in this work to denser flows, in order to create an efficient and versatile tool, able to describe gas-particle flow over the full range of particle-phase volume fractions. Although not discussed here, the same approach for approximating the kinetic equation is applicable to polydisperse gas-particle flows by coupling a multi-component kinetic equation with the fluid solver. Such as approach naturally accounts for particle-particle collisions between like and unlike particles, as well as differences in the fluid drag depending on the particle type.

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