Numerical simulation of turbulent gas-particle flow in a riser using a quadrature-based moment method

Alberto Passalacqua  
*Iowa State University*, albertop@iastate.edu

Rodney O. Fox  
*Iowa State University*, rofox@iastate.edu

Follow this and additional works at: http://lib.dr.iastate.edu/cbe_conf

Part of the Biochemical and Biomolecular Engineering Commons, and the Catalysis and Reaction Engineering Commons

Recommended Citation

http://lib.dr.iastate.edu/cbe_conf/6

This Conference Proceeding is brought to you for free and open access by the Chemical and Biological Engineering at Iowa State University Digital Repository. It has been accepted for inclusion in Chemical and Biological Engineering Conference Presentations and Proceedings by an authorized administrator of Iowa State University Digital Repository. For more information, please contact digirep@iastate.edu.
Numerical simulation of turbulent gas-particle flow in a riser using a quadrature-based moment method

A. Passalacqua and R. O. Fox

Department of Chemical and Biological Engineering, Iowa State University, Ames, IA 50011-2230, USA
† albertop@iastate.edu and rofox@iastate.edu

Keywords: Quadrature-based moment method, gas-particle flow, riser flow

Abstract

Gas-particle flows are used in many industrial applications in the energy, oil and gas fields, such as coal gasification, production of light hydrocarbons by fluid catalytic cracking, catalytic combustion and different treatments aiming to reduce or eliminate pollutants. The particle phase of a gas-particle flow is described by analogy to a granular gas, by finding an approximate solution of the kinetic equation in the velocity-based number density function. In the recent past, many studies have been published on the mathematical modeling of gas-particle flows using hydrodynamic models (e.g. Enwald et al. 1996), where Navier-Stokes-type equations are solved to describe the particle phase as a continuum, computing its stress tensor using moment closures from kinetic theory (Gidaspow 1994). These closures, however, are obtained assuming that the flow is dominated by collisions and near equilibrium, which corresponds to considering a very small particle-phase Knudsen number. This assumption leads to inconsistencies and erroneous predictions of physical phenomena when these models are applied to dilute fluid-particle flows, where rarefaction effects are not negligible. In these flows, the wall Knudsen layers extend inside the bulk of the fluid, and cannot be accounted for with the simple addition of partial-slip boundary conditions. Recently Desjardin et al. (2008) showed that two-fluid models are unable to correctly capture particle trajectory crossing, seriously compromising their ability to correctly describe any velocity moment for finite Stokes numbers. These authors clarified that the particle segregation captured by two-fluid models for finite Knudsen numbers is artificially high due to their mathematical formulation, which leads to the formation of delta-shocks. In order to overcome these shortcomings, Fox (2008) developed a third-order quadrature-based moment method for dilute gas-particle flows, which has been successfully coupled to a fluid solver to compute dilute and moderately dilute gas-particle flows by Passalacqua et al. (2010) in two dimensions. These authors validated their model against Euler-Lagrange and two-fluid simulations. In this work, the fully coupled quadrature-based fluid-particle code described in Passalacqua et al. (2010) is applied to simulate turbulent gas-particle flow in the riser described by He et al. (2009), using a three-dimensional configuration. This application shows the predictive capabilities and the robustness of the quadrature-based moment method to predict the behavior of gas-particle flows in accordance with experiments (He et al. 2009).

Nomenclature

Roman symbols

\( C_D \) drag coefficient
\( d_p \) particle diameter (m)
\( e_p \) particle-particle restitution coefficient
\( e_w \) particle-wall restitution coefficient
\( f \) distribution function
\( F \) force acting on each particle (N)
\( g \) gravitational acceleration (m/s\(^{-1}\))
\( g_0 \) radial distribution function
\( I \) identity matrix

Kn Knudsen number
Ma Mach number
\( m_p \) particle mass (kg)
\( n_\alpha \) quadrature weight
\( M_{fp} \) momentum exchange due to drag (kg/(m\(^2\) s\(^2\)))
\( M_{ljk} \) velocity moment ((m/s\(^4\)))
\( p \) pressure (Pa)
Pr Prandtl number
Re Reynolds number
Stokes number

time (s)

velocity (m/s)


time (s)

quadrature abscissa (m/s)

particle velocity (m/s)

position vector

Greek symbols

volume fraction

set of equilibrium moments

granular temperature (m^2/s^2)

dynamic viscosity (Pa s)

density (kg/m^3)

particle-phase stress tensor components

fluid-phase stress tensor components

collision time (s)

Subscripts

f Fluid

p Particle

Superscripts

f Fluid

p Particle

Introduction

Gas-particle flows in risers have been the topic of extensive research in order to develop reliable computational models capable of describing their peculiarities. Generally speaking, two kind of approaches are possible to describe the particle phase: the Lagrangian approach, where each particle trajectory is resolved independently, applying fundamental laws of mechanics, and the Eulerian approach, in which the particle phase is described by transport equations of moments of the particle velocity distribution function. The computational convenience and the absence of statistical noise characteristic of Eulerian models made them very attractive both for research and applications, and significant effort to improve their formulation has been spent in the last two decades. Syamlal and Gidaspow (1985); Gidaspow (1986) developed hydrodynamic models for CFB reactors, accounting for heat transfer and introducing a normal stress modulus for the particulate phase. Gidaspow et al. (1989); Tsuo and Gidaspow (1990) adopted the Wen and Yu (1966) drag correlation in their model, and properly predicted flow regimes typical of the circulating fluidised bed risers. Sinclair and Jackson (1989); Sinclair (1997) showed that a hydrodynamic model is able to properly predict the behavior of a gas-solid flow in a riser if all the interactions between the phases are accounted for, and correlated these interactions to the averaged and fluctuating components of the phase velocity fields. Sinclair and Jackson (1989) also developed the first stationary hydrodynamic model able to predict the particulate phase stresses through the kinetic theory of the granular flow, as a function of the particle fluctuating energy (granular energy). Pita and Sundaresan (1991) modified the Sinclair and Jackson (1989) model and validated it against Bader et al. (1988) experimental data, showing its high sensitivity to the value of the restitution coefficient, whose reduction may lead to a wrong prediction of the particles segregation patterns inside the duct. Lounge et al. (1991) introduced a one-equation turbulence model to describe the gas phase turbulence, and adopted standard wall-functions for the zone near the wall. Gidaspow and Therdthianwong (1993) adopted a zero-equation closure for the gas phase turbulence. Ocone et al. (1993) extended the work of Sinclair and Jackson (1989) to arbitrarily inclined ducts, accounting for the effects of particles sliding and rotation. Bolio et al. (1995) adopted a low-Reynolds two-equation \( \varepsilon - \kappa \) model for the gas phase, to eliminate the need for wall functions. Hrenya and Sinclair (1997) studied the influence of turbulence both on the transport equations and on the kinetic theory closure equations, leading to a reformulation of the dissipation term of the granular energy, which resulted in a reduced sensitivity of the model to the value of the particle restitution coefficient. Benyahia et al. (2000); Arastoopour (2001) simulated a FCC riser using the kinetic theory of granular flow, neglecting the gas-phase turbulence. Peirano and Leckner (1998); Peirano et al. (2002); De Wilde et al. (2002) adopted a model that couples a two-equation turbulence model with a set of two equations for the particulate-phase turbulent kinetic energy and for the gas-particle velocity correlation Gidaspow and Therdthianwong (1993); Samuelsberg and Hjertager (1996); Mathiesen et al. (2000); Huilin and Gidaspow (2003); Huilin et al. (2006) introduced the Smagorinsky (1963) sub-grid stress model to describe the turbulence of the gas phase following the principles of large-eddy simulation. Recently Ibsen et al. (2004) compared discrete methods and multi-fluid models in circulating fluidised beds. Zeng and Zhou (2006) developed a two-scale second-order moment particle turbulence model for dense gas-particle flows. Moreau et al. (2009) proposed a new large-eddy simulation approach for particle-laden turbulent flows in the framework of the Eulerian formalism for inertial particles. He et al. (2009) performed experiments in a riser with mono-dispersed particles and compared the measurements with the results of numerical simulations performed using the La-
grangian discrete particle model (DPM) approach.

In this work we present the results of the simulations of the same system considered by He et al. (2009) obtained with a fully three-dimensional implementation of the quadrature-based moment method developed by Fox (2008) and coupled with a fluid solver by Passalacqua et al. (2010). Results are compared to experimental data, statistics of the particle phase are computed and dimensionless parameters such as the particle-phase Mach, Knudsen and Stokes numbers of the flow are examined.

Model description

Fluid-phase governing equations. The fluid phase, assumed to be incompressible and isothermal, is described by a continuity and a momentum equation as in traditional two-fluid models (Drew 1971; Gidaspow 1994; Enwald et al. 1996). The fluid continuity equation has the form

$$\frac{∂}{∂t} (α_f ρ_f) + \nabla \cdot (α_f ρ_f \mathbf{U}_f) = 0,$$

and the fluid momentum equation is

$$\frac{∂}{∂t} (α_f ρ_f \mathbf{U}_f) + \nabla \cdot (α_f ρ_f \mathbf{U}_f \mathbf{U}_f) = \nabla \cdot (α_f \mathbf{τ}_f) - \alpha_t \nabla p + α_f ρ_f \mathbf{g} + \mathbf{M}_{fp}.$$

where $α_f$, $ρ_f$, $\mathbf{U}_f$ are the fluid-phase volume fraction, density and mean velocity, $\mathbf{M}_{fp}$ represent the momentum exchange term due to the drag between the fluid and particle phases, and $\mathbf{g}$ is the gravitational acceleration vector.

The stress tensor $τ_f$ is

$$τ_f = μ_f \left( \nabla \mathbf{U}_f + (\nabla \mathbf{U}_f)^T \right) - \frac{2}{3} μ_f \left( \nabla \cdot \mathbf{U}_f \right) \mathbf{I},$$

where $μ_f$ is the dynamic viscosity of the fluid and $\mathbf{I}$ the unit tensor.

Particle-phase governing equations. The particle phase is described in analogy to a gas made of smooth, mono-disperse, non-cohesive spheres. Its governing equation is represented by a kinetic equation for the particle number density function $f(t, x, \mathbf{v})$ (Chapman and Cowling 1961; Cercignani et al. 1994; Struchtrup 2005)

$$\frac{∂f}{∂t} + \mathbf{v} \cdot \frac{∂f}{∂x} + \frac{∂}{∂\mathbf{v}} \cdot \left( \frac{\mathbf{F}}{m_p} \right) = \mathbb{C},$$

where $\mathbf{F}$ is the force acting on each particle, including gravity and drag, and $\mathbb{C}$ represents the rate of change in the number density function due to binary collisions between the particles.

The collision term $\mathbb{C}$ is described using the Bhatnagar-Gross-Krook (BGK) collision operator (Bhatnagar et al. 1954):

$$\mathbb{C} = \frac{1}{τ_c} \left( f_{eq} - f \right),$$

where $τ_c$ is the collision time and $f_{eq}$ is the equilibrium distribution function, extended to account for inelastic collisions:

$$f_{eq} = \frac{M^0}{[\det (2π\lambda)]^{1/2}} \exp \left( -\frac{1}{2} (v_i - U_{p,i}) \lambda^{-1} (v_j - U_{p,j}) \right),$$

where $λ^{-1}$ is the inverse of the $μ$ matrix $λ$, defined by

$$λ = γ ω^2 Θ_p \mathbf{I} + (γ ω^2 - 2 γ ω + 1) \mathbf{σ}$$

with $γ = 1/Pr$, $ω = (1 + e)/2$, $M^0$ the number density of particles (zero-order moment), $U_p$, $v_i$ mean particle velocity, $e$ the restitution coefficient, $Θ_p$ the granular temperature, and $σ$ the velocity covariance matrix. In this work $γ = 1$, so that $Pr = 1$ in the standard BGK model (Struchtrup 2005).

In this work, following Fox (2008); Passalacqua et al. (2010), a set of twenty moments of $f$ up to third order is considered. Each moment is defined through integrals of the distribution function as

$$M^0 = \int f dv, \quad M^1_i = \int v_i f dv,$n

$$M^2_{ij} = \int v_i v_j f dv, \quad M^3_{ijk} = \int v_i v_j v_k f dv.$$

Transport equations for the moments are obtained by applying the definition (8) to both sides of the kinetic equation, leading to (Fox 2008)

$$\frac{∂M^0}{∂t} + \frac{∂M^1_i}{∂x_i} = 0,$n

$$\frac{∂M^1_i}{∂t} + \frac{∂M^2_{ij}}{∂x_j} = A^1_i,$n

$$\frac{∂M^2_{ij}}{∂t} + \frac{∂M^3_{ijk}}{∂x_k} = C^2_{ij} + A^2_{ij},$$

$$\frac{∂M^3_{ijk}}{∂t} + \frac{∂M^4_{ijkl}}{∂x_l} = C^3_{ijk} + A^3_{ijk},$$

where $A^1_i$, $A^2_{ij}$ and $A^3_{ijk}$ are the source terms due to the acceleration acting on each particle, and $C^2_{ij}$ and $C^3_{ijk}$ are those due to the collision operator.

The set of transport equations (9) is not closed, because each equation contains the spatial flux of the moments of order immediately higher, and the source terms due to the force and to collisions. Gaussian quadrature
formulæ are used to provide closures for these source terms as a function of a set of weights \( n_\alpha \) and abscissas \( U_\alpha \). Weights and abscissas are computed from the set of transported moments by means of an inversion algorithm. Following Fox (2008), a set of eight weights and abscissas per each velocity component is used.

The moments can be computed as a function of the quadrature weights and abscissas using the definition (8):

\[
M^0 = \sum_{\alpha=1}^{\beta} n_\alpha,
\]

\[
M_i^1 = \sum_{\alpha=1}^{\beta} n_\alpha U_{\alpha i},
\]

\[
M_i^2 = \sum_{\alpha=1}^{\beta} n_\alpha U_{\alpha i} U_{\alpha j},
\]

\[
M_i^3 = \sum_{\alpha=1}^{\beta} n_\alpha U_{\alpha i} U_{\alpha j} U_{\alpha k}.
\]

The source terms due to drag and gravity are computed as

\[
A_i^1 = \sum_{\alpha=1}^{\beta} n_\alpha \left( \frac{F_D}{m_p} + g_i \right) U_{j\alpha},
\]

\[
A_i^2 = \sum_{\alpha=1}^{\beta} n_\alpha \left[ \left( \frac{F_D}{m_p} + g_i \right) U_{j\alpha} + \left( \frac{F_{\alpha j}}{m_p} + g_j \right) U_{i\alpha} \right],
\]

\[
A_i^3 = \sum_{\alpha=1}^{\beta} n_\alpha \left[ \left( \frac{F_D}{m_p} + g_i \right) U_{j\alpha} U_{k\alpha} + \left( \frac{F_{\alpha j}}{m_p} + g_j \right) U_{k\alpha} U_{i\alpha} + \left( \frac{F_{\alpha k}}{m_p} + g_k \right) U_{i\alpha} U_{j\alpha} \right].
\]

The drag force terms are given by

\[
F_D^\alpha = \frac{m_p}{\tau_\alpha} (U_\alpha - U_{\alpha}) = K_{fp,\alpha} (U_\alpha - U_{\alpha}).
\]

The drag time, computed for each velocity abscissa, is calculated as

\[
\tau_\alpha^D = \frac{4d_p^2 \rho_p}{3\alpha f m_p C_D(Re_p, \alpha_f) Re_p},
\]

where the particle Reynolds number is defined for each abscissa by

\[
Re_p = \frac{\rho_p d_p |U_\alpha - U_{\alpha}|}{\mu_t},
\]

and the drag coefficient \( C_D \) is modeled according to Wen and Yu (1966):

\[
C_D(Re_p, \alpha_f) = \frac{24}{\alpha_f Re_p} \left[ 1 + 0.15(\alpha_f Re_p)^{0.687} \right] \alpha_f^{-2.65}.
\]

The source terms in the moment transport equations due to collisions are given by

\[
C^2_{ij} = \frac{\alpha_p}{\tau_c} (\lambda_{ij} - \sigma_{ij}),
\]

\[
C^3_{ijk} = \frac{1}{\tau_c} (\Delta_{ijk} - M_{ijk}^3),
\]

in which the collision time is defined by

\[
\tau_c = \frac{\pi^{1/2} d_p}{12 \alpha_p \Theta_p \Theta_p^{1/2}},
\]

with \( \Theta_p \) defined in terms of the moments by

\[
\Theta_p = \frac{1}{3} (\sigma_{11} + \sigma_{22} + \sigma_{33}),
\]

\[
\sigma_{11} = \frac{M_{11}^2}{M_0^2} - \left( \frac{M_1^1}{M_0^0} \right)^2,
\]

\[
\sigma_{22} = \frac{M_{22}^2}{M_0^2} - \left( \frac{M_1^1}{M_0^0} \right)^2,
\]

\[
\sigma_{33} = \frac{M_{33}^2}{M_0^2} - \left( \frac{M_1^1}{M_0^0} \right)^2.
\]

The radial distribution function of Carnahan and Starling (1969) is adopted:

\[
g_0 = \frac{1}{1 - \alpha_p} + \frac{3 \alpha_p}{2 (1 - \alpha_p)^2} + \frac{\alpha_p^2}{2 (1 - \alpha_p)^3}.
\]

The moment spatial fluxes are represented by the second term on the left-hand side of (9), and are computed according to their kinetic definition (Perthame 1990; Desjardin et al. 2008; Fox 2008) in order to ensure the realizability of the set of moments.

**Boundary conditions.** Boundary conditions for the moment transport equations are specified in terms of the quadrature approximation, as shown in Fox (2008); Paschalacqua et al. (2010). The specular reflective condition at walls is defined as

\[
\begin{pmatrix}
    n_\alpha \\
    U_{\alpha 1} \\
    U_{\alpha 2} \\
    U_{\alpha 3}
\end{pmatrix}_{i=0} = \begin{pmatrix}
    n_\alpha / \epsilon_w \\
    -\epsilon_w U_{\alpha 1} \\
    -\epsilon_w U_{\alpha 2} \\
    U_{\alpha 3}
\end{pmatrix}_{i=1},
\]

where \( \epsilon_w \) is the restitution coefficient for collisions between a particle and the wall, and \( i = 0 \) represents the wall, assumed to be along the second direction in the considered reference frame. Periodic boundary conditions are imposed by enforcing the periodicity on the set of weights and abscissas.
Figure 1: Schematic representation of the riser considered in He et al. (2009). The hashed area represents the actual portion of the riser considered in the simulations.

Test case description

The model presented above has been implemented in the CFD code MFIX (Syamlal et al. 1993; Syamlal 1998) as detailed in Passalacqua et al. (2010), and is validated here against the experimental measurements in a gas-particle flow riser, with mono-disperse particles, realized by He et al. (2009). The experimental setup used in this reference is constituted by a riser column of rectangular section, as schematically represented in Fig. 1. The dimensions of the riser and the properties of the fluid and particle phases are reported in Table 1.

Simulation setup

The computational domain considered in this work represents only a portion of the whole riser examined in the experiments of He et al. (2009), in the center of the column, with a height L, as represented by the dashed volume in Fig. 1. Periodic boundary conditions were imposed at the top and at the bottom of the computational domain, while no-slip conditions were used for the fluid phase at the wall, and reflective conditions with restitution coefficient $e_w$ were used for the particle phase.

Table 1: Dimensions of the riser and flow properties

<table>
<thead>
<tr>
<th>Variable</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>W</td>
<td>0.05</td>
<td>m</td>
</tr>
<tr>
<td>H</td>
<td>1.5</td>
<td>m</td>
</tr>
<tr>
<td>D</td>
<td>0.015</td>
<td>m</td>
</tr>
<tr>
<td>L</td>
<td>0.30</td>
<td>m</td>
</tr>
<tr>
<td>$d_p$</td>
<td>335.0</td>
<td>µm</td>
</tr>
<tr>
<td>$\rho_p$</td>
<td>2500.0</td>
<td>kg/m³</td>
</tr>
<tr>
<td>$e_p$</td>
<td>0.97</td>
<td>–</td>
</tr>
<tr>
<td>$G_s$</td>
<td>10.0</td>
<td>kg/(m³·s)</td>
</tr>
<tr>
<td>$\rho_f$</td>
<td>1.2</td>
<td>kg/m³</td>
</tr>
<tr>
<td>$\mu_f$</td>
<td>1.8 · 10^{-5}</td>
<td>Pa·s</td>
</tr>
<tr>
<td>$U_f$</td>
<td>2.3</td>
<td>m/s</td>
</tr>
<tr>
<td>$U_i$</td>
<td>2.7</td>
<td>m/s</td>
</tr>
</tbody>
</table>

The fluid-phase mass flux has been imposed to match the mean particle mass flux $G_s$, by adapting the pressure gradient along the height of the computational domain.

The grid density used in the simulations, taken from the work of He et al. (2009), is 25 grid points along W, 60 along L and 10 along D. Simulations were performed with an adaptive time stepping, based on the convergence of the fluid-phase residuals (Syamlal et al. 1993), on the QMOM CFL condition, on the particle collision time and the drag time. Simulations are performed for a total of 10 s of simulation time, while time averages are computed on the last 5 s of simulation time. Since the domain is periodic, averages are computed assuming the $z$ direction to be homogeneous, and considering a symmetry plane, located at $W/2$, normal to the $x$ direction. The RMS values are found by subtracting the time-averaged values from the instantaneous fields, and time averaging the square of the differences. The final RMS value are then the square root of time-averaged square differences.

The fluid-phase equations are solved with an iterative procedure based on the SIMPLE (Patankar 1980; Ferziger and Peric 2002), and coupled with the QMOM equations using the partial elimination algorithm (Spalding 1980), as shown in Passalacqua et al. (2010). The second-order scheme with superbee limiter was used to discretize the fluid-phase equations. As convergence criterion for all the variable of the fluid-phase, a reduction of the residuals below $10^{-4}$ was required to consider the solution converged.

Results and discussion

An example of the instantaneous solids volume fraction field at $t = 8$ s obtained in the simulation performed using the quadrature-based moment method is reported.
in Fig. 2. It can be seen that particles segregated at the walls of the riser, forming ensembles at higher volume fraction, which tends to move downward, since their weight wins the resistance exerted by the fluid. As explained in Passalacqua et al. (2010), the flow evolves from the uniform initial conditions through an intermediate state where particles, due to the reflective conditions at the walls, tend to originate two vertical stripes parallel to the walls, with lower particle concentration. In these stripes the fluid accelerates, and the difference in shear causes the flow to become unstable. The instability quickly propagates to the whole flow, leading to the segregation of particles typically observed in riser flows.

The time-averaged volume fraction, shown in Fig. 3 (experimental data is not available for this quantity), is lowest in the center of the flow and highest at the walls, which is typical of core-annular flow.

Results of the time-averaged vertical component of the velocity obtained in the simulation performed using the quadrature-based moment method are reported in Fig. 4 and compared with the experiments of He et al. (2009). In all the reported plots, $x = 0$ represents the channel centerline, and $x = 0.025$ m indicates the channel wall. The predicted values of the axial velocity show a core-annular behavior, with negative values at the wall, indicating particles fall in that region of the system, and positive values in the center of the riser. Results are in acceptable agreement with the experimental measurements of He et al. (2009), and similar to those obtained by the same authors performing Lagrangian simulations.

The convergence of the averages is considered satisfactory, in spite of the relatively short averaging time, since the values of the time-averaged velocity along the $x$ direction (Fig. 5), are approximately zero, as expected when the flow reaches the steady-state condition. The root-mean-square (RMS) of the vertical component of the velocity of the particle phase is reported in Fig. 6, and is in qualitative agreement with the experiments of He et al. (2009), but not in quantitative agreement. Both the experimental and the computational profiles show a minimum at the riser centerline, and the maximum value in proximity of the wall, but at a certain distance from it. The RMS velocity in the $x$ direction, reported in Fig. 7 is in quantitative agreement with the experimental data. Differences in the numerical predictions compared to the experimental data might depend on the simplified numerical configuration used in the simulation, where only one portion of the system is considered, and periodicity is assumed in the axial direction. Further reasons that could explain the differences are the choice of the drag law, as well as other sub-models used in the numerical model, and the systematic errors in the experimental measurements (He et al. 2009).

The time-averaged granular temperature is reported in Fig. 8. (Note that the granular temperature is not related to the RMS velocity statistics!) The values of $\Theta_p$
present a minimum at the wall of the channel, where the collision frequency is higher due to higher particle concentration, due to particle segregation, and a maximum in the core of the riser, where the flow is dilute and collisions are not predominant, as shown in Fig. 10. Before proceeding to consider the behavior of the Knudsen number in detail, it is worth noticing that the flow is in transonic conditions, meaning that there are parts of the computational domain where the particle velocity is above or equal to the local particle-phase ‘speed of sound’ \( \text{Ma} > 1 \), and other parts of the system where the particle velocity is below the the local value of the speed of sound \( \text{Ma} < 1 \). This is evident from the values of the time-averaged local particle Mach number \( \text{Ma} = |\mathbf{U}_p|/\Theta_p^{1/2} \) in Fig. 9, which shows the \( \text{Ma} \) is approximately between \( 6 \times 10^{-3} \) and 1.8. Under these conditions, two regimes are present in the system. Where \( \text{Ma} < 1 \), the flow is dominated by diffusive processes, regulated by the local value of the granular temperature, which has to be used to compute the characteristic velocity in this regime. When \( \text{Ma} > 1 \), the flow is dominated by convective phenomena, meaning that the transport of properties is mainly due to the convective transport of particles more than to diffusive phenomena, and the granular temperature has to be replaced by the local mean velocity magnitude in the definition of the characteristic velocity of the flow. The two zones are separated by a dashed line in Fig. 9. Since the flow undergoes a transition between two different regimes, the definition of the Knudsen number has to be modified according to the region where it is computed, following Kogan (1969), so that

\[
\text{Kn} = \begin{cases} \sqrt{\frac{\tau_c}{\pi}} & \text{Ma} < 1 \\ \frac{\sqrt{\tau_c |\mathbf{U}_p|}}{L} & \text{Ma} > 1 \end{cases}
\]

(22)

where the collision time is given by

\[
\tau_c = \frac{d_p}{12 \rho_0 a_p} \frac{\Theta_p}{\sqrt{\Theta_p}}.
\]

(23)

The values of the Knudsen number, computed assuming \( L = 2WD/(W + D) \), according to the definition of hydraulic diameter of the riser, are reported in Fig. 10. The diagram shows the flow transitions from the slip regime, where \( 0.01 < \text{Kn} < 0.1 \) (Bird 1994), in the region adjacent to the wall, to a more rarified regime (transitional regime) in the center of the riser, where non-equilibrium phenomena are expected to happen. The two regions are separated by the dotted line. The lower value of Kn at the wall is justified by the higher particle concentration in that region of the system, which leads to higher values of the collision frequency, making the flow locally dominated by collisions. It is worth noticing that if an hydrodynamic model (Gidaspow 1994; Enwald et al. 1996), derived in the hypothesis of nearly zero Knudsen number (Continuum regime, \( \text{Kn} < 0.01 \)) were used to perform the simulation, the adoption of partial slip boundary conditions (Johnson and Jackson 1987) would have been necessary to describe the behavior of the flow in the zone adjacent

---

**Figure 4:** Time-averaged \( z \) component of the particle velocity.

**Figure 5:** Time-averaged \( x \) component of the particle velocity.
to the walls, where $Kn < 0.1$, however the model would have deviated from the correct behavior in the center of the riser, where higher values of the Knudsen number are present, and higher-order approximations of the kinetic equation than the hydrodynamic are necessary.

The Stokes number profile is reported in Fig. 11, and reports values between 66.1 and 123.5, which indicate particles reaction to changes in the local conditions of the fluid flow are not instantaneous, but delayed and, since the flow is dilute, might lead to particle trajectory crossing. As pointed out in Desjardin et al. (2008), such phenomenon cannot be predicted by hydrodynamic models, since they only consider moments up to the second order, and define only one local velocity in each computational cell, whereas multiple local velocities are necessary to be able to capture the discontinuous velocity field that originates when particle trajectory crossing occurs. This becomes clear considering the particle velocity distribution function. The hydrodynamic models are obtained assuming equilibrium or nearly-equilibrium conditions, imposing that the velocity distribution is Maxwellian. When particle trajectory crossing occurs faster particles pass slower particles, locally the velocity becomes multi-valued and the distribution function strongly deviates from the equilibrium condition, originating discontinuities in the velocity field, which cannot be described under the hydrodynamic hypothesis, since single-valued velocity is assumed in these models. Hydrodynamic models hypothesize the flow is always dominated by collisions, and predict unphysical accumulation of particles (delta-shocks), as shown in Desjardin et al. (2008), who simulated the behavior of particles in Taylor-Green flow at different Stokes numbers, and compared the solutions obtained with Lagrangian simulations, Eulerian quadrature-based simulations, and hydrodynamic models.

**Conclusions**

A portion of a riser of a circulating fluidized bed have been simulated using a third-order quadrature-based moment method in a fully three-dimensional numerical setup, showing the robustness and the capability of the quadrature-based moment method for this kind of applications. Results for the time-averaged mean particle velocity were found in satisfactory agreement with the experimental results in spite of the simplifying assumptions made in the simulation about the periodicity of the computational domain. RMS velocities were found in qualitative agreement with experiments, but not in quantitative agreement, for what concerns the vertical component of the velocity.

Characteristic dimensionless parameters of the particle flow were examined. The Mach number showed that the particle flow is in transonic conditions, with the subsonic region adjacent to the wall. The values of the local Knudsen number pointed out the flow is in a condition across two regimes: the slip regime (zone adjacent to the wall) and the transition regime (center of the channel), indicating that the adoption of hydrodynamic models in
Figure 8: Time-averaged granular temperature profile.

Figure 9: Time-averaged Mach number profile.

Figure 10: Time-averaged Knudsen number profile.

Figure 11: Time-averaged Stokes number profile.
such a regime would be inappropriate. This was further confirmed by considering the local values of the Stokes number, which clarified that particles do not immediately react to the fluid flow, and can originate particle trajectory crossing wherever the flow is not dominated by collisions (high $Kn$).

Future work will involve the simulation of systems with more realistic boundary conditions and geometries than those considered in the present work and the examination of denser flow conditions. Additionally, idealized simulations in domains with periodic conditions in all the spatial directions will be performed to further investigate the formation of clusters and the conditions that lead to flow instabilities at the base of the particle segregation.

Acknowledgements

This work has been supported by the National Energy Technology Laboratory of the U.S. Department of Energy under the award number DE-FC26-07NT43098.

References


