ON THE SUB-GRID TWO-FLUID SIMULATION OF GAS-SOLID RISER FLOWS

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Abstract. *At present, computational experiment represents the most promising way for sub-grid investigation in gas-solid flows and, the most practical approach to modeling the concerning flow comes from the so called Eulerian or two-fluid models. The up to date literature presents only a few sub-grid simulations of gas-solid flows in risers applying two-fluid modeling, including Agrawal et al. (2001) and Andrews IV et al. (2005). Those authors applied a particulate size typical of catalytic cracking fluidized bed reactors (75 μm). In the present work, results are presented for a particulate size typical of circulating fluidized bed coal combustors (520 μm). Simulations were performed for this late situation as well as for Agrawal's conditions. The results of the simulations are compared to each other, and an evaluation is advanced regarding the validity of the current approach for generating sub-grid correlations for riser flows.*

Keywords*: two-fluid modeling, sub-grid simulation, gas-solid flow, riser*

1. INTRODUCTION

The gas-solid flow in risers of real scale circulating fluidized bed reactors develops in very large domains. As a consequence, current computational limitations impose that any whole domain numerical simulation of the process is necessarily performed in very coarse spatial meshes. However, in the search for more precise predictions, simulations can be performed in partial domains thereby allowing more refined spatial meshes. If both, the spatial and the temporal meshes are sufficiently enough refined, so that the whole physics of the flow is captured, a simulation is usually referred to as numerical direct simulation (NDS). In this case closure relations are required only at a micro-scale level, and all of the meso and macro-scales of the flow are resolved.

Gas-solid flows in risers are characterized by intense and dynamical formation and dissipation of coherent structures of particles, generally known as clusters, strands or streamers. Such structures may be as large as the size of the column and, according to Agrawal et al. (2001), as small as about ten times the size of the particles. Sharma et al. (2000) found the life time of clusters in a typical riser flow to be of the order of 10^{-2} seconds. When coarse meshes both spatial and temporal are applied in a simulation, clusters whose spatial and temporal scales are smaller than the respective mesh sizes are filtered, and sub-grid models become required.

It is clear that NDS can not be applied to real risers. Despite temporal meshes can be applied that are adequate for NDS, the same is not true regarding spatial meshes. In a whole domain simulation, only the spatial macro-scale is resolved, and additional information is needed so as to recover spatial meso-scale effects filtered by the numerical meshes. Thereby, besides the micro-scale information, additional spatial meso-scale information is also required. A simulation taking into account the meso-scale behavior by means of sub-grid models may be addressed to as a large cluster simulation (LCS), in analogy to the large eddy simulation (LES) applied in turbulence modeling. While LES requires sub-grid models to recover the effects of non-resolved eddies, LCS requires sub-grid models to recover the effects of non-resolved clusters.

The development of closure sub-grid models for LCS is an open question on modeling and simulation of gas-solid flows. Unfortunately, as remarked by Sundaresan (2000), the state of the art in experimental techniques does not provide enough resolution for investigation into the meso-scale of gas-solid flows. A possibility on the theoretical front would be to apply sub-grid models developed for mono-phase turbulent flows. This, however, was ruled out by Agrawal et al. (2001), who showed the meso-scale viscosity of a solid phase to be inversely proportional to the macro-scale deformation rate, which is contrary to what happens in mono-phase turbulent flows. Sundaresan (2000) points out that, at present, computational experiment represents the most promising way for sub-grid investigation in gas-solid flows. The author observes, in addition, that the most practical approach to modeling the concerning flow comes from the so called Eulerian or two-fluid models.

The up to date literature presents only a few sub-grid simulations of gas-solid flows in risers applying two-fluid modeling. As far as the sub-grid approach is concerned, the works of Agrawal et al. (2001) and Andrews IV et al. (2005) may be taken as references. Agrawal et al. (2001) presented an analysis of their sub-grid predictions pointing out the potential of the results for generating sub-grid correlations. Andrews IV et al. (2005) extended the analysis of Agrawal and co-workers, and actually produced sub-grid correlations from their computational experiments. Those correlations were then used in a LCS simulation of a riser flow, and the results were considered by the authors to be inadequate for comparisons to experiment. Both, Agrawal et al. (2001) and Andrews IV et al. (2005) concluded that their results are ad-hoc first approximations, and that much needs to be done before suitable sub-grid correlations can be derived.

The present work intends to be a contribution to the discussion on the above matter. Agrawal et al. (2001) and Andrews IV et al. (2005) applied a particulate size typical of catalytic cracking fluidized bed reactors (75 μm), where high density flows are practiced. In the present work results are presented for a particulate size typical of circulating fluidized bed coal combustors (520 μm), where dilute flows are practiced. Simulations are presented for this late situation as well as for Agrawal's conditions. Then, the results of the simulations are compared to each other, and an evaluation is advanced regarding the validity of the current approach for generating sub-grid correlations for gas-solid flows in risers.

2. TWO-FLUID MODELING APPROACH

Multiphase flow two-fluid models stand on the major hypothesis of continuum for all of the phases, no matter fluid or particulate. The phases are treated as inter-penetrating dispersed continua in thermodynamic equilibrium. The theory of two-fluid models has been developed by many researchers. Some classical reference works on this matter are those due to Anderson and Jackson (1967), Ishii (1975), Drew (1983), Gidaspow (1994) and Enwald et al. (1996). The construction of a two-fluid model departs from integral conservative balances over a control volume comprising all of the phases. The theorems of Leibniz and Gauss are applied over the integral balances providing local instantaneous conservative equations for the different phases, and jump conditions describing interface interactions among phases. The interfaces in inter-penetrating dispersed flows are very dynamical and chaotic, which makes the local instantaneous formulations unsolvable. In view of that, averaging procedures are applied over the local instantaneous formulation providing averaged equations. In the averaged formulation, the effects of many interfaces are treated in average as a field effect describing the action of one phase over the others. Volume averaging, time averaging or ensemble averaging are usually applied giving rise to averaged equations which are similar in form, but different as for the interpretation of the averaged variables. Whatever the averaging procedure applied, the final conservative equations are mathematically identical to the local instantaneous equations, except for the presence of field terms accounting for the interactions among phases.

To complete a two-fluid model, closure laws must be formulated. Those laws provide correlations for viscous stress tensors, viscosities, pressures and drag. All of the phases are usually treated as Newtonian-Stokesian fluids. Pressures and viscosities of particulate phases are obtained from either empiricism or theory. Interface drag is accounted for from semi-empirical correlations. Other interface forces such as lift and added mass are usually disregarded.

When the interest is turned to sub-grid simulation, closure laws must be defined which provide descriptions at the micro-scale of the flow. Regarding gas-solid flows, the current state of the art does not include micro-scale experimental information, so that the so called kinetic theory of granular flows (KTGF) is usually applied. This is an analogy with the kinetic theory of dense gases, which is modified to account for the inelastic particle collisions characteristic of gas-solid flows (Lun et al., 1984). Just like the kinetic energy fluctuations of molecules defines the thermodynamic temperature, the kinetic energy fluctuations of particles defines the so called granular temperature. The same way, a pseudo-thermal energy is defined in analogy with the thermodynamic thermal energy, and the granular temperature is obtained from a pseudo-thermal energy conservation balance. Concepts of granular pressure and viscosities are advanced, and those parameters may be correlated to granular temperature just like pressure and viscosity can be correlated to thermodynamic temperature.

In this work periodic boundary conditions are applied. This means that both the phases penetrate a boundary of the domain and reappear at a parallel similar opposing boundary, and vice versa. In consequence, all of the variables of the flow through parallel similar boundaries are made locally and instantly identical. When replacing a conventional entrance condition by a periodic condition, however, the flow driven force which balances gravity is removed, causing the flow to accelerate in the gravitational direction until a new balance is found where gravity and buoyancy balance drag, and the particulate free fall terminal velocity is met. Such a flow condition is not suitable for riser flows, and a realistic compensation of gravity must be found. This is usually done by imposing an extra gas phase pressure gradient in the vertical direction. Agrawal et al. (2001) and Andrews IV et al. (2005) considered this gradient to exactly match the gravity acting on the suspension. This assumption is brought from previous studies on the instabilities that develop in unforced granular materials when the inelasticity of the collisions among particles is accounted for, which ultimately leads to the formation of clusters (see, for instance, Goldhirsch et al., 1993, and Tan and Goldhirsch, 1997). Those studies clearly stand for quasi static regimes, where particulates arrange themselves in low velocity suspensions. It is believed, however, that the clustering mechanism that prevails is also relevant to rapid gas-solid flows (Tan and Goldhirsch, 1997). In the present work this assumption is followed, just as previously done by both Agrawal et al. (2001) and Andrews IV et al. (2005).

A formulation of the two-fluid model including closure laws based on the KTGF (Gidaspow, 1994; Syamlal et al., 1993, Agrawal et al., 2001), and including gravity compensation for applying periodic boundary conditions, comprises:

Gas phase continuity

$$\frac{\partial}{\partial t}\left(\rho_g \alpha_g\right)+\vec{\nabla}\cdot\left(\rho_g \alpha_g \vec{U}_g\right)=0 \tag{1}$$

Solid phase continuity

$$\frac{\partial}{\partial t}\left(\rho_s \alpha_s\right)+\vec{\nabla}\cdot\left(\rho_s \alpha_s \vec{U}_s\right)=0 \tag{2}$$

Gas phase momentum

$$\frac{\partial}{\partial t}\left(\rho_g \alpha_g \vec{U}_g\right)+\vec{\nabla}\cdot\left(\rho_g \alpha_g \vec{U}_g \vec{U}_g\right)=-\alpha_g\left(\vec{\nabla}P_g+\vec{\nabla}P_g^*\right)+\vec{\nabla}\cdot\left(\alpha_g \overline{\overline{\tau}}_g\right)+\rho_g \alpha_g \vec{g}+\beta\left(\vec{U}_s-\vec{U}_g\right) \tag{3}$$

Solid phase momentum

$$\frac{\partial}{\partial t}\left(\rho_s \alpha_s \vec{U}_s\right)+\vec{\nabla}\cdot\left(\rho_s \alpha_s \vec{U}_s \vec{U}_s\right)=-\alpha_s\left(\vec{\nabla}P_g+\vec{\nabla}P_g^*\right)-\vec{\nabla}\left(P_s\right)+\vec{\nabla}\cdot\left(\alpha_s \overline{\overline{\tau}}_s\right)+\rho_s \alpha_s \vec{g}-\beta\left(\vec{U}_s-\vec{U}_g\right) \tag{4}$$

Volumetric continuity

$$\alpha_g+\alpha_s=1 \tag{5}$$

Interface drag function

$$\beta=150\frac{\alpha_s^2 \mu_g}{\alpha_g (d_p \varphi_s)^2}+1.75\frac{\rho_g \alpha_s \left|v_g-v_s\right|}{(d_p \varphi_s)} \quad \text{for } \alpha_s>0.2 \qquad \text{(Ergun, 1952)} \tag{6}$$

$$\beta=\frac{3}{4}C_{Ds}\frac{\rho_g \alpha_s \alpha_g \left|v_g-v_s\right|}{(d_p \varphi_s)}\alpha_g^{-2.65} \quad \text{for } \alpha_s\leq 0.2 \qquad \text{(Wen and Yu, 1966)} \tag{7}$$

$$\text{where } C_{Ds}=\begin{cases}\dfrac{24}{Re_P}(1+0.15\cdot Re_p^{0.687}) & \text{for} \quad Re_p<1000\\ 0.44 & \text{for} \quad Re_p\geq 1000\end{cases} \qquad \text{(Rowe,1961)} \tag{8}$$

$$Re_p=\frac{\left|v_g-v_s\right| d_p \rho_g \alpha_g}{\mu_g} \tag{9}$$

Granular temperature (Syamlal et al., 1993)

$$\Theta=\left(\frac{-K_1\alpha_s tr\left(\overline{\overline{D}}_s\right)+\sqrt{K_1^2 tr^2\left(\overline{\overline{D}}_s\right)\alpha_s^2+4K_4\alpha_s\left[K_2 tr^2\left(\overline{\overline{D}}_s\right)+2K_3 tr\left(\overline{\overline{D}}_s^2\right)\right]}}{2\alpha_s K_4}\right)^2 \tag{10}$$

$$\text{where } \overline{\overline{D}}_s=\tfrac{1}{2}\left[\vec{\nabla}\vec{U}_s+\left(\vec{\nabla}\vec{U}_s\right)^T\right] \tag{11}$$

$$K_1=2(1+e)\rho_s g_0 \tag{12}$$

$$K_2=\frac{4d_p \rho_s (1+e)\alpha_s g_0}{3\sqrt{\pi}}-\frac{2}{3}K_3 \tag{13}$$

$$K_3=\frac{d_p \rho_s}{2}\left\{\frac{\sqrt{\pi}}{3(3-e)}\left[1+0.4(1+e)(3e-1)\alpha_s g_0\right]+\frac{8\alpha_s g_0(1+e)}{5\sqrt{\pi}}\right\} \tag{14}$$

$$K_4=\frac{12\left(1-e^2\right)\rho_s g_0}{d_p\sqrt{\pi}} \tag{15}$$

$$g_0 = \frac{3}{5}\left[1-\left(\frac{\alpha_s}{\alpha_{s,max}}\right)^{1/3}\right]^{-1} \tag{16}$$

Viscous stress tensor ($k = s, g$)

$$\bar{\bar{\tau}}_k = \mu_k\left[\vec{\nabla}\vec{U}_k + \left(\vec{\nabla}\vec{U}_k\right)^T\right] + \left(\lambda_k - \tfrac{2}{3}\mu_k\right)\left(\vec{\nabla}\cdot\vec{U}_k\right)\bar{\bar{I}} \tag{17}$$

where $\mu_g = \text{constant}$ (18)

$$\lambda_g = 0 \tag{19}$$

$$\mu_s = \frac{4}{5}\alpha_s^2\rho_s d_p g_0 (1+e)\left(\frac{\Theta}{\pi}\right)^{1/2} \tag{20}$$

$$\lambda_s = \frac{4}{3}\alpha_s^2\rho_s d_p g_0 (1+e)\left(\frac{\Theta}{\pi}\right)^{1/2} \tag{21}$$

Solid phase pressure

$$P_s = \alpha_s\rho_s\Theta\left[1 + 2(1+e)g_0\alpha_s\right] \tag{22}$$

Gravity compensation (for periodic boundaries)

$$\vec{\nabla}P_g^* = \left(\rho_s\alpha_s + \rho_g\alpha_g\right)\vec{g} \tag{23}$$

The algebraic expression for the granular temperature given in Eq. (10) was derived by Syamlal et al. (1993) by assuming that the pseudo-thermal energy is locally generated by viscous stress and dissipated by inelastic collisions.

The symbols in Eqs. (1) to (23) stand for:

C_D	- drag coefficient, non-dimensional
d_p	- particle diameter, m
e	- solid phase restitution coefficient, non-dimensional
$\vec{g}$	- gravity acceleration, m/s^2
g_0	- radial distribution function, non-dimensional
$\bar{\bar{I}}$	- unit tensor
P	- pressure, N/m^2
$\vec{\nabla}P_g^*$	- extra gas phase pressure gradient for exactly matching the gravity on the suspension, N/m^3
Re_p	- Reynolds number, non-dimensional
t	- time, s
$\vec{U}$	- average velocity vector, m/s
u, v, w	- velocity components in the x, y, z directions, m/s

Greek

α	- volume fraction, m_k^3/m^3
$\alpha_{s,max}$	- solid volume fraction at packing, m_s^3/m^3
β	- gas-solid friction coefficient, kg/m^{3}s
Θ	- granular temperature, m^2/s^2
λ	- bulk viscosity, Ns/m^2
μ	- dynamic viscosity, Ns/m^2
ρ	- density, kg/m^3
$\bar{\bar{\tau}}$	- viscous stress tensor, N/m^2
φ	- particle sphericity, non-dimensional

Subscripts

g	- gas phase
k	- either gas or solid phases
s	- solid phase

The complex set of partial differential non-linear coupled equations of the two-fluid models can only be solved through numerical procedures. In this work, the numerical model available in the software CFX (CFX, 2004) is used. An element-based finite volume discretization method is followed. Non-structured meshes are applied in Cartesian coordinate system. Uniform hexahedral mesh elements are used. The median method is applied to define control volumes over which the conservative equations are integrated to obtain the discretized equations. The discretization of convective terms is performed through a second order high resolution interpolation scheme. The discretization of diffusive and other terms is performed through the second order central differencing scheme. Time discretization is performed through a first order interpolation scheme. The discretized equations are solved implicitly through a direct method applying matrix inversion. As a consequence, couplings such as pressure x velocity, and drag, are straightly solved, and iteration is only required to overcome non-linearities.

3. SIMULATIONS SET UP

A 2cm x 2cm x 8cm vertical hexahedral domain is considered, applying 1mm x 1mm x 1mm uniform hexahedral numerical meshes. Two different cases are simulated, whose operating conditions are described in Table 1. Case I is taken from Agrawal et al. (2001), and represents a situation typical of catalytic cracking. Case II is taken from Milioli (2006), and represents a situation typical of coal combustion. A solid volume fraction of 0.05 is imposed for both the cases through the initial conditions. Table 1 also brings the numerical conditions that were applied.

The time steps of 10^{-4} and $5x10^{-5}$ seconds which were applied in cases I and II, respectively, are suitable for sub-grid simulations. The expected time scale of clusters of the order of 10^{-2} seconds (following Sharma et al., 2000) is expected to be fully captured in both the cases. For case II a particulate size of 520 μm is applied, and the smaller clusters on the flow are expected not to be larger than 5.2 mm (following Agrawal et al., 2001). Therefore, the applied spatial mesh of 1mm x 1mm x 1mm is adequate for the sub-grid simulation of this case. The same can not be said of case I, where the smaller clusters are expected to be as small as 0.75mm. In this case, a numerical mesh finer than the currently applied would be necessary. However, the computational cost of such a mesh would be prohibitive in view of the computational resources which are available.

Table 1. Cases, operating conditions, numerical conditions.

Domain	Initial conditions
2 cm x 2 cm x 8cm	$u_g = v_g = w_g = 0$ m/s
Boundary conditions	$u_s = v_s = w_s = 0$ m/s
Periodic at entrance and exit	$\alpha_s = 0.05\ \mathrm{m_s^3/m^3}$
Free slip at walls	
Mesh	Solid phase restitution coefficient
32000 cubic cells (1mm x 1mm x 1mm)	$e = 0.9$
35721 nodes	
rms for convergence	
1 x 10^{-5}	
Case I	Case II
$d_p = 75$ μm	$d_p = 520$ μm
$\rho_s = 1500$ kg/m^3	$\rho_s = 2620$ kg/m^3
$\rho_g = 1.3$ kg/m^3	$\rho_g = 1.1614$ kg/m^3
$\mu_g = 1.8 \times 10^{-5}$ Pa.s	$\mu_g = 1.82 \times 10^{-5}$ Pa.s
Time step = 1 x 10^{-4} s	Time step = 5 x 10^{-5} s

4. RESULTS AND DISCUSSION

Figure 1 shows grayscale plots of solid volume fraction in an axial section of the domain, for cases I (particulate of 75 μm, 1500 kg/m^3) and II (particulate of 520 μm, 2620 kg/m^3). The effects of particle size/density over the topology of the flow are quite clear. The smaller and lighter particulate of case I gives rise to a more refined structure formed of smaller clusters. In case II, otherwise, much larger structures are formed.

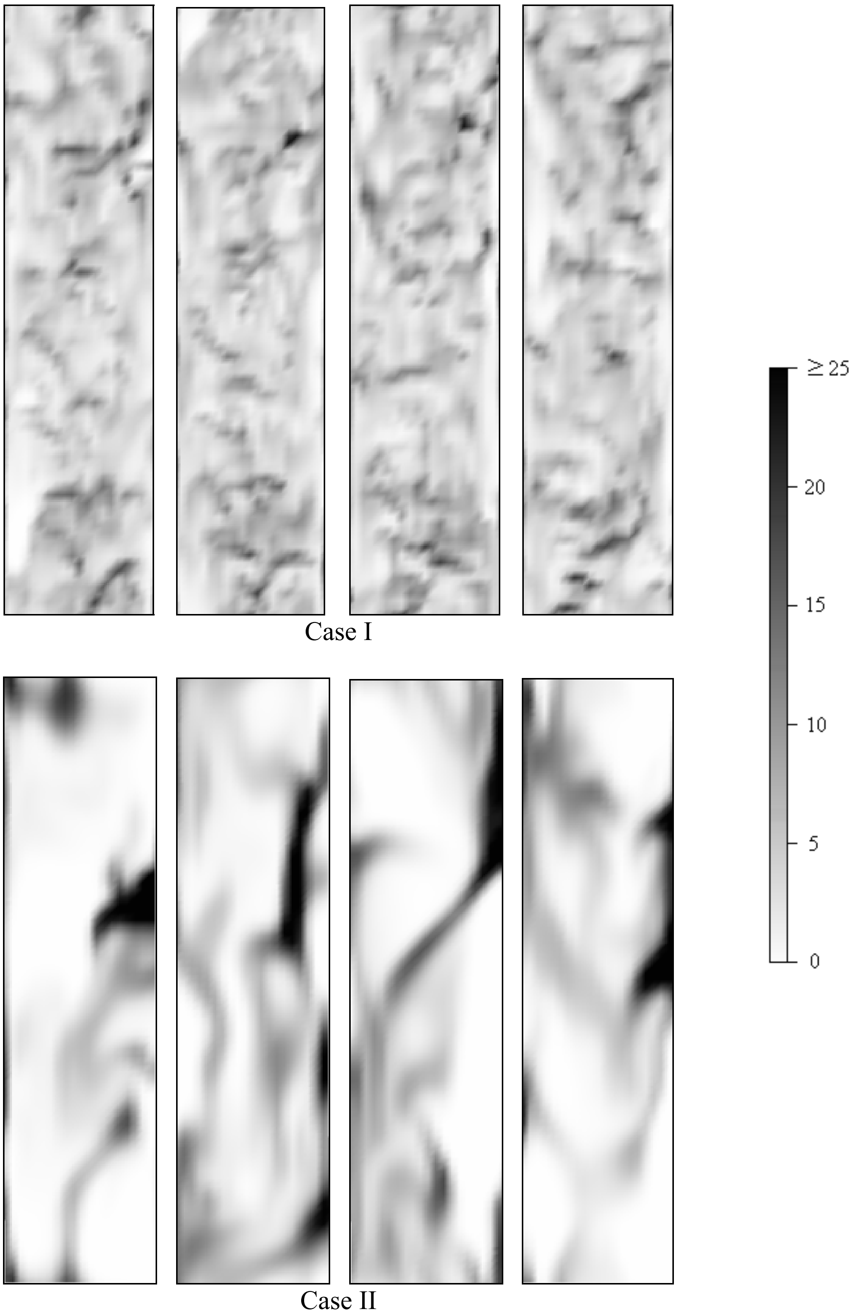
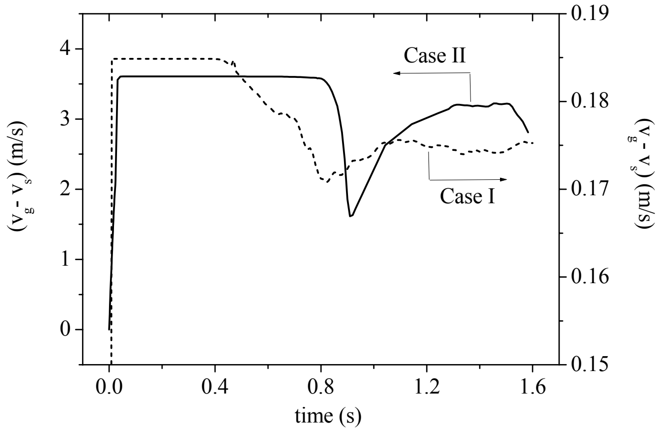


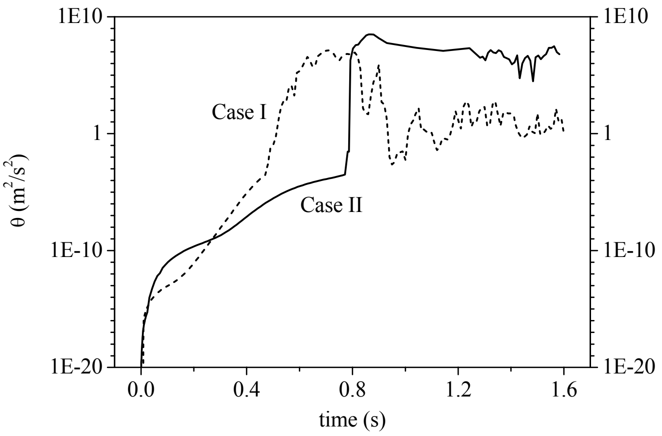
Figure 1. Grayscale plots of solid volume fraction in an axial section of the domain, for cases I and II (real scales).

Figure 2 presents the transient behavior of the slip velocity (Fig. 2a) and the granular temperature (Fig. 2b), averaged over the whole domain, for cases I and II. After starting from rest, the slip velocity quickly grows up and stand unchanged while the flow is kept uniform. When clusters start to be formed, the slip velocity starts to oscillate around averages characteristic of the quasi steady state flow regime. This behavior is observed in both cases I and II. However, the order of magnitude of the slip velocity, and the order of magnitude of its time changing, result higher for the larger and denser particles of case II (520 μm, 2620 kg/m^3) in comparison to the smaller and lighter particles of case I (75 μm, 1500 kg/m^3). Various effects may significantly contribute to that behavior. Drag, solid phase pressure and solid phase viscosities are quite dependent on particle size and/or density. Granular temperature is also very dependent on those parameters. Besides, the gravity compensation procedure imposes a higher extra pressure gradient for the larger and heavier particulate.

The transient behavior of the granular temperature, for both cases, also shows oscillations leading to the quasi steady state flow regime. Granular temperature departs from zero at rest to reach very high values, and then starts to oscillate around the well defined averages characteristic of the quasi steady state flow regime. A dramatic change in this settled average, of several orders of magnitude, is observed between the cases, showing how the calculation of granular temperature is dramatically affected by particle size and density.



(a)



(b)

Figure 2. Transient behavior of parameters averaged over the whole domain, for cases I and II. (a) slip velocity; (b) granular temperature.

Figure 3 presents a comparison of time averaged cross section profiles of gas velocity (Fig. 3a), solid velocity (Fig. 3b), slip velocity (Fig. 3c), solid volume fraction (Fig. 3d), and granular temperature (Fig. 3e), for cases I and II. All the velocity profiles are very flat, which is a consequence of the free-slip condition that was enforced at the walls for both the phases. Gas and solid velocities for case II result much higher than those for case I. The slip velocity also results much higher for case II. Negative profiles of solid velocity were found in both cases, which frontally opposes reality, where the average net flow is upward. Solid volume fraction oscillates about averages which are similar for both the cases. This was expected since an average solid volume fraction was enforced equal for both the cases through the initial conditions, and considering that the gravity over the gas-solid suspension was compensated through an extra gas pressure gradient in the momentum equations. On the absence of gravity acting on the suspension, the domain average phase concentrations are expected to remain constant.

In both cases, the granular temperature throughout the section oscillates between lower and higher values by orders of magnitude. The oscillations were even more intense for the larger/heavier particulate of case II. This dramatic effect requires further investigation, and suggests that the KTGF model used to determine granular temperature requires revision.

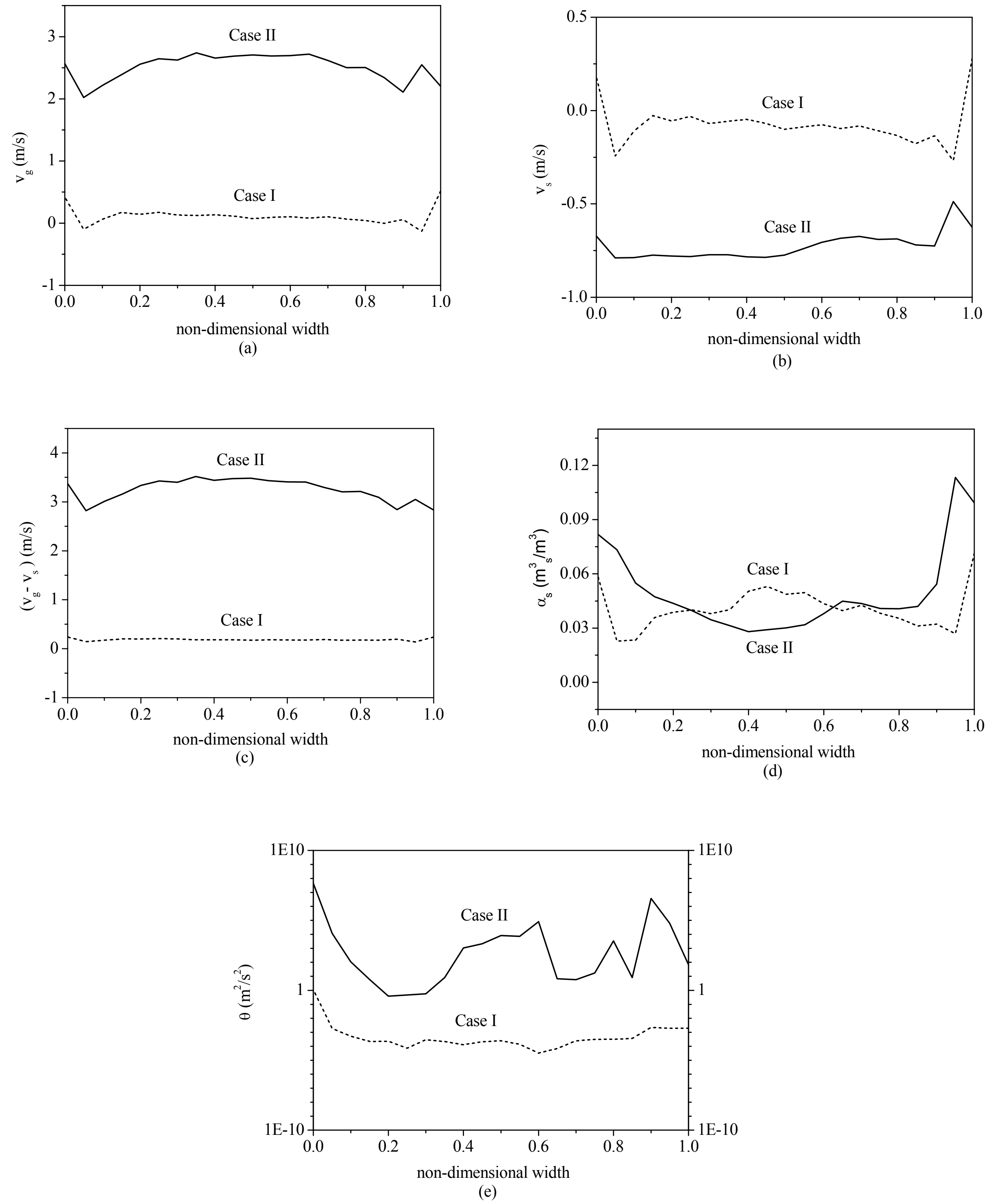


Figure 3. Time averaged profiles of gas axial velocity (a), solid axial velocity (b), slip velocity (c), solid volume fraction (d), and granular temperature (e) over the central line through a cross section of the domain at 4 cm above entrance.

5. CONCLUSIONS

The present simulations must be addressed regarding their validity for describing the flow which actually develops in the sub-grid domain of a rapid gas-solid flow. In the simulations periodical boundary conditions where applied in the axial direction, so that the flow driven force was removed. To recover from that, an extra gas phase pressure gradient was introduced which exactly balanced the gravity acting on the gas-solid suspension. As a result, in both the cases considered, what was actually simulated was a low velocity gas-solid suspension predominantly defined by gravity and drag. A primordial question to be answered is on whether this low velocity field can be treated as a broad flow independent structure which periodically repeats itself in all directions inside of a rapid gas-solid stream of a real riser.

In the present simulations slip velocities were found which are in the correct order of magnitude as compared to those for rapid gas-solid flows. However, even though the difference between the gas and the solid phase axial velocities seem realistic, the phase velocities themselves are not. Negative average solid phase axial velocities were found. This means that the average solid phase mass flow is downwards, which is obviously unrealistic.

It seems that new thinking is required so that more realistic sub-grid flows can be found. An attempt to find out more realistic velocity fields can be made by imposing an extra gas phase pressure gradient chosen to exceed that required to balance the gravity acting on the suspension. As a consequence, the flow is expected to accelerate and a new balance shall be found at a superior level of gas velocity. This issue is currently on the agenda.

6. ACKNOWLEDGEMENTS

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