A SUB-GRID TWO-FLUID SIMULATION OF A TYPICAL GAS-SOLID RISER FLOW

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Abstract. *Two-fluid modeling is widely applied to simulate gas-solid flows in risers. Current simulations are either large cluster simulations performed in coarse numerical meshes, or sub-grid simulations performed in reduced domains. In this work, two different simulations are considered for a typical gas-solid riser flow: a coarse grid and a sub-grid simulation. The coarse grid simulation applies empirical data for the viscosity of the solid phase, and a empirical correlation for the solid phase pressure; a small scale real riser domain is considered using a coarse tetrahedral numerical mesh of 9.4 mm average edge. The sub-grid simulation applies theoretical correlations derived from the kinetic theory of granular flows to define pressure and viscosities of the solid phase; a small size domain is considered under periodic boundary conditions, using a refined numerical mesh. The predictions of the coarse grid and the sub-grid simulations are compared to each other, and to experiment. Then, the accuracy of the simulations is addressed in view of the experimental data.*

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

1. INTRODUCTION

Two-fluid models are extensively applied to simulate gas-solid flows in risers. However, the very large domains of real risers and prohibitively high computational costs impose the application of very coarse spatial meshes. As a consequence, the scales of the flow which are smaller than the numerical mesh can not be resolved, and sub-grid models become required. The current simulations of risers must be seen, therefore, as large cluster simulations (LCS), which are conceptually similar to the large eddy simulations (LES) applied in turbulence modeling.

A huge problem related to LCS applied to gas-solid flows in risers is that the current literature presents no sub-grid models valid for those flows. In view of that, many researchers apply empirical data or semi-empirical correlations to deal with models' parameters such as solid phase viscosity, solid phase pressure and drag (Tsuo and Gidaspow, 1990; Miller and Gidaspow, 1992; Mathiesen et al., 2000; Zhang and Van der Hyden, 2001; Huilin and Gidaspow, 2003; Cabezas-Gómez and Milioli, 2003; Georg, 2005; Milioli, 2006; among others). Other researchers apply theoretical correlations derived from the kinetic theory of granular flows (KTGF) (Gidaspow, 1994; Agrawal et al., 2001; Andrews IV et al., 2005; Jiradilok et al., 2006; among others). Unlike a formulation including empirical data or semi-empirical correlations, a formulation based on KTGF is suitable for sub-grid simulations, as done by Agrawal et al. (2001) and Andrews IV et al. (2005).

Owing to its gas molecular analog nature, KTGF allows the prediction of the meso-scale of the flow through numerical direct simulation (NDS) since it provides a description of the micro-scale of the flow. LCS can only resolve the macro-scales of the flow, requiring meso-scale data to be provided through sub-grid modeling which, at its turn, requires micro-scale modeling. Macro-scale comprises all the scales of the flow that can be resolved by coarse meshes; meso-scale comprises all the scales that are filtered by the coarse meshes; while micro-scale is that immediately smaller than the smallest scale of the flow. Concerning the particulate, the smaller scale in a riser gas-solid flow is the size of the smaller clusters that are formed. According to Agrawal et al. (2001), such size is about ten times the particulate diameter. Therefore, a sub-grid simulation must apply mesh sizes smaller then ten times the diameter of the particles.

In this work two different simulations are considered for a typical gas-solid riser flow. The first is a LCS simulation for a small scale real riser, performed in a coarse grid applying empirical data for the viscosity of the solid phase, and a empirical correlation for the solid phase pressure. The second is a sub-grid simulation applying theoretical correlations derived from KTGF, performed in a small size domain under periodic boundary conditions, and using a refined numerical mesh. The predictions of the coarse grid and the sub-grid simulations are compared to each other, and to experiment. Then, the accuracy of the simulations is addressed in view of experimental data.

2. TWO-FLUID MODELS FOR GAS-SOLID FLOWS

Two-fluid models for gas-solid flows comprise a set of averaged conservative equations plus a number of closure relations (see, for instance, Anderson and Jackson, 1967; Ishii, 1975; Drew, 1983; Gidaspow, 1994; and Enwald et al., 1996). Closure laws provide correlations for viscous stress tensors, viscosities, pressures and drag. The phases are usually treated as Newtonian-Stokesian fluids, while pressures and viscosities of solid phases are obtained from either

empiricism or theory, and interface drag is accounted for from semi-empirical correlations. The basic governing equations of the two-fluid models applied to gas-solid flows are (Gidaspow, 1994):

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

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

Solid phase momentum

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

Volumetric continuity

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

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

$$\overline{\overline{\tau}}_k=\mu_k\left[\vec{\nabla}\vec{U}_k+\left(\vec{\nabla}\vec{U}_k\right)^T\right]+\left(\lambda_k-\tfrac{2}{3}\mu_k\right)\left(\vec{\nabla}\cdot\vec{U}_k\right)\overline{\overline{I}} \tag{6}$$

where $\mu_g = \text{constant}$ (7)

$$\lambda_g=0 \tag{8}$$

Interface drag function

$$\beta=150\frac{\alpha_s^2 \mu_g}{\alpha_g\left(d_p \varphi_s\right)^2}+1.75\frac{\rho_g \alpha_s\left|v_g-v_s\right|}{\left(d_p \varphi_s\right)} \quad \text{for } \alpha_s>0.2 \quad \text{(Ergun, 1952)} \tag{9}$$

$$\beta=\frac{3}{4}C_{Ds}\frac{\rho_g \alpha_s \alpha_g\left|v_g-v_s\right|}{\left(d_p \varphi_s\right)}\alpha_g^{-2.65} \quad \text{for } \alpha_s \le 0.2 \quad \text{(Wen and Yu, 1966)} \tag{10}$$

$$\text{where } C_{Ds}=\begin{cases}\dfrac{24}{Re_P}\left(1+0.15\cdot Re_p^{0.687}\right) & for \quad Re_p<1000\\ 0.44 & for \quad Re_p \ge 1000\end{cases} \quad \text{(Rowe,1961)} \tag{11}$$

$$Re_p=\frac{\left|v_g-v_s\right| d_p \rho_g \alpha_g}{\mu_g} \tag{12}$$

2.1. Closure for coarse grid simulation

This is a conventional formulation of the two-fluids models for gas-solid flows, where pressure and viscosities of solid phases are brought from empiricism. A contact effect of particle to particle collisions defines solid phase pressure. Similarly, a contact effect of particle to particle attrition defines solid phase viscosity. Both contact effects are affected by kinetics and dumping effects. Regarding the solid phase pressure, the kinetics effect is generally disregarded, and the particle to particle collisions are modeled in terms of an elasticity modulus correlated from experiment (Gidaspow and Ettehadieh, 1983). Regarding the solid phase viscosities, only the particle to particle attrition and dumping affects are significant, and simplified momentum balances combined with empirical data are applied (Tsuo and Gidaspow, 1990; Miller and Gidaspow, 1992). The coarse grid simulation presented in this work, which was performed by Milioli (2006), applies a constant solid phase viscosity empirically obtained by Tsuo and Gidaspow (1990). The concerning closure relations are (Gidaspow, 1994; Milioli, 2006):

Solid phase viscosities

$$\mu_s = \text{constant} \tag{13}$$

$$\lambda_s = 0 \tag{14}$$

Solid phase pressure

$$\vec{\nabla}(P_s) = G\vec{\nabla}\alpha_s \tag{15}$$

$$\text{where } G = exp\left[-20\left(\alpha_g - 0.62\right)\right] \text{ (Gidaspow and Ettehadieh, 1983)} \tag{16}$$

2.2. Closure for sub-grid simulation

Here the kinetic theory of granular flows (KTGF) is applied to define micro-scale solid phase viscosities and pressure. KTGF 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.

Sub-grid simulations are required to be applied in reduced computational domains, and a reduced domain must be applied which is representative of the flow in a real riser. To accomplish for that, periodic boundary conditions are applied in the flow axial direction. This means that both the phases penetrate a boundary of the domain and reappear at a parallel similar opposing boundary, and vice versa. When applying periodic boundary conditions in the gravitational direction, 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, which exactly matches the gravity acting on the suspension (Agrawal et al., 2001; Andrews IV et al., 2005).

Accounting for the above, a sub-grid simulation includes, in addition to Eqs. (1) to (10), the following formulation (Gidaspow, 1994; Syamlan et al., 1993, Agrawal et al., 2001):

Granular temperature (Syamlal et al., 1993)

$$\Theta = \left(\frac{-K_1\alpha_s tr\left(\overline{\overline{D}}_s\right) + \sqrt{K_1^2 tr^2\left(\overline{\overline{D}}_s\right)\alpha_s^2 + 4K_4\alpha_s\left[K_2 tr^2\left(\overline{\overline{D}}_s\right) + 2K_3 tr\left(\overline{\overline{D}}_s^2\right)\right]}}{2\alpha_s K_4} \right)^2 \tag{17}$$

$$\text{where } \overline{\overline{D}}_s = \frac{1}{2}\left[\vec{\nabla}\vec{U}_s + \left(\vec{\nabla}\vec{U}_s\right)^T\right] \tag{18}$$

$$K_1 = 2(1+e)\rho_s g_0 \tag{19}$$

$$K_2 = \frac{4d_p\rho_s(1+e)\alpha_s g_0}{3\sqrt{\pi}} - \frac{2}{3}K_3 \tag{20}$$

$$K_3 = \frac{d_p\rho_s}{2}\left\{\frac{\sqrt{\pi}}{3(3-e)}\left[1+0.4(1+e)(3e-1)\alpha_s g_0\right] + \frac{8\alpha_s g_0(1+e)}{5\sqrt{\pi}}\right\} \tag{21}$$

$$K_4 = \frac{12\left(1-e^2\right)\rho_s g_0}{d_p\sqrt{\pi}} \tag{22}$$

$$g_0 = \frac{3}{5}\left[1-\left(\frac{\alpha_s}{\alpha_{s,max}}\right)^{1/3}\right]^{-1} \tag{23}$$

Solid phase viscosities

$$\mu_s = \frac{4}{5}\alpha_s^2 \rho_s d_p g_0 (1+e)\left(\frac{\Theta}{\pi}\right)^{1/2} \tag{24}$$

$$\lambda_s = \frac{4}{3}\alpha_s^2 \rho_s d_p g_0 (1+e)\left(\frac{\Theta}{\pi}\right)^{1/2} \tag{25}$$

Solid phase pressure

$$P_s = \alpha_s \rho_s \Theta[1 + 2(1+e) g_0 \alpha_s] \tag{26}$$

Gravity compensation: in the momentum Eqs. (3) and (4) $\vec{\nabla} P_g$ must be replaced by $\vec{\nabla} P_g + \vec{\nabla} P_g^*$, where

$$\vec{\nabla} P_g^* = (\rho_s \alpha_s + \rho_g \alpha_g)\vec{g} \tag{27}$$

The algebraic expression for the granular temperature given in Eq. (17) 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 (27) 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
G - particle-particle elasticity modulus, N/m^2
$\bar{\bar{I}}$ - 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, non-dimensional
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

2.3. Numerical procedure

The simulations in this work were performed with the numerical model available in the software CFX (CFX, 2004). An element-based finite volume discretization method is followed. 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. Non-structured meshes are applied in Cartesian coordinate system. Tetrahedral non-uniform mesh elements were used in the coarse grid simulation, while uniform hexahedral mesh elements were used in the sub-grid simulation.

3. SIMULATIONS SET UP

Two different simulations are considered in the present work: a coarse grid and a sub-grid simulation. The coarse grid simulation was previously performed by Milioli (2006), for Luo's experimental conditions (Luo, 1987). A riser of 7.62 cm i.d. and 5.56 m high was considered, applying a particulate of 520 μm diameter and 2620 kg/m^3 density, and gas inlet at 4.979 m/s. The sub-grid simulation was performed for the same particulate size of 520 μm. Considering this particulate size, 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.

Tables 1 and 2 bring the operational set up for both the coarse grid and the sub-grid simulations.

Table 1. Set up for the coarse grid simulation (Milioli, 2006).

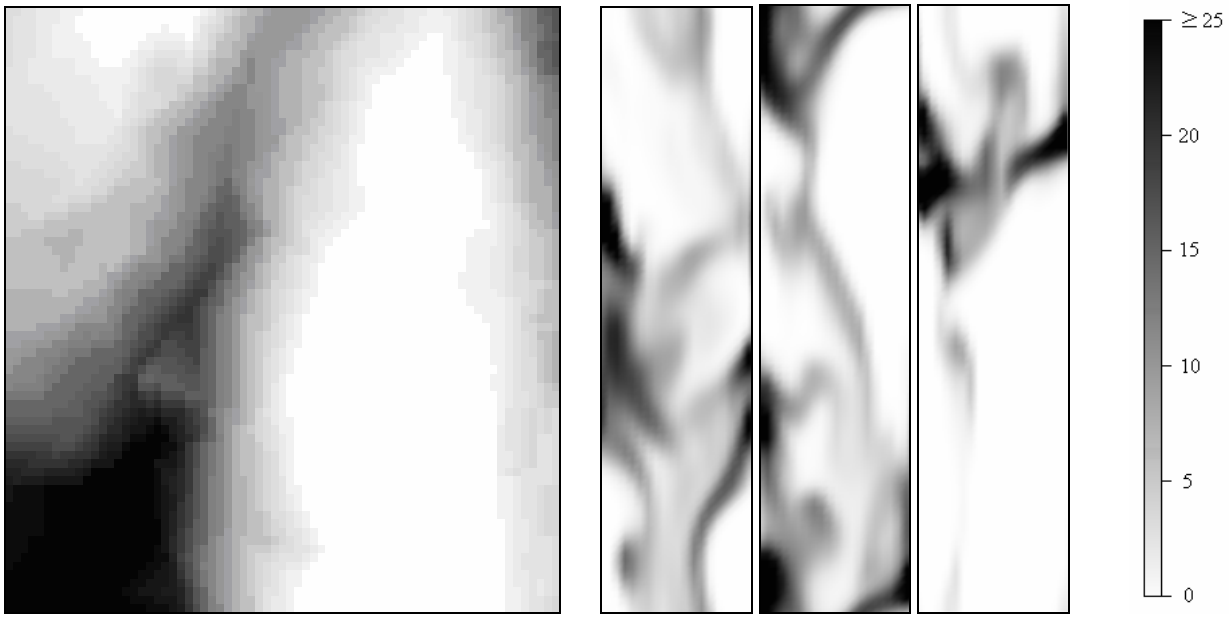
Domain	Boundary conditions
7.62cm i.d. x 5.56m high	Inlet
Particle and gas properties	$u_g = 0$ m/s
$d_p =$ 520 μm	$v_g = 4.979$ m/s
$\rho_s = 2620$ kg/m^3	$w_g = 0$ m/s
$\rho_g = 1.1614$ kg/m^3	$u_s = 0$ m/s
$\mu_g = 1.82$ x 10^{-5} N.s/m^2	$v_s = 0.386$ m/s
Initial conditions: as in the inlet, except	$w_s = 0$ m/s
$\alpha_s = 0.38$ m$_s^3$/m^3	$\alpha_s = 0.0246$ m$_s^3$/m^3
Mesh	Outlet
206229 tetrahedrals (average edge 9.4 mm)	Locally parabolic
42029 nodes	$P_g = 15880$ N/m^2
Time step	Walls
1 x 10^{-4} s	No-slip for the gas phase
rms for convergence	Free slip for the solid phase
1 x 10^{-5}	

Table 2. Set up for the sub-grid simulation.

Domain	Initial conditions
2cm x 2cm x 8cm	$u_g = v_g = w_g =$ 0 m/s
Particle and gas properties	$u_s = v_s = w_s = 0$ m/s
$d_p =$ 520 μm	$\alpha_s = 0.05$ m$_s^3$/m^3
$\rho_s = 2620$ kg/m^3	Mesh
$\rho_g = 1.1614$ kg/m^3	32000 cubic cells (1mm x 1mm x 1mm)
$\mu_g = 1.82$ x 10^{-5} N.s/m^2	35721 nodes
Solid phase restitution coefficient	Time step
$e = 0.9$	5 x 10^{-5} s
Boundary conditions	rms for convergence
Periodic at inlet and outlet	1 x 10^{-5}
Free slip at walls	

4. RESULTS AND DISCUSSION

Figure 1 presents grayscale plots of solid volume fraction in an axial section of the domain, for the present sub-grid simulation and the coarse grid simulation of Milioli (2006). Its is clear that the refined mesh of the sub-grid simulation catches a much more refined structure of clusters which can not be captured by the coarse grid simulation.



Coarse grid simulation (Milioli, 2006) Sug-grid simulation

Figure 1. Grayscale plots of solid volume fraction in an axial section of the domain, for the present sub-grid simulation and the coarse grid simulation of Milioli (2006) (real scales).

Figure 2 shows time averaged profiles of gas axial velocity (Fig. 2a), solid axial velocity (Fig. 2b), slip velocity (Fig. 2c), and solid volume fraction (Fig. 2d), for the coarse and the sub-grid simulations, in comparison to experimental data. The coarse grid simulation was performed by Milioli (2006), while the empirical data were produced by Luo (1987). The profiles in the figures stand for a central line through the cross section of the domain at 4 cm above entrance for the sub-grid simulation, and at 3.4 m above entrance for the experimental data and for the coarse grid simulation.

All the figures show great discrepancies of both the simulations to each other, and to experiment. The gas velocity profiles of Fig. 2a show a better prediction of the coarse grid simulation close to the walls, but a very poor prediction far from the walls. The sub-grid simulation produced a better qualitative flat profile far from the walls, but quantitatively quite deviated. The solid phase velocities shown in Fig. 2b are tremendously deviated from experiment for both the predictions. It is interesting to note that a fully negative profile of solid phase velocity was found in the sub-grid simulation, which frontally opposes reality, where the average net flow is upward. Both the simulations seem to catch the slip velocity correctly close to the walls, but quite deviated in the core (Fig. 2c). As seen in Fig. 4d, the solid phase volume fraction was highly overestimated by both the simulations, even though they correctly captured the expected profile behavior.

The above results are not surprising. The coarse grid simulation did not considered any suitable sub-grid model, so that it would not be reasonable to suppose that their predictions could accurately represent experiment. The sub-grid simulation considered a very small domain, so that the larger clusters that ultimately define the flow topology could not be caught. There is also a great deal of uncertainty regarding the correlations derived from the kinetic theory of granular flows, which require further validation. The present results make it clear that only a large cluster simulation (LCT) can possibly provide accurate predictions which, unfortunately, are currently out of reach owing to the lack of suitable sub-grid models.

Table 3 shows averaged parameters for the sub-grid and coarse grid simulations, in comparison to experiment. The sub-grid results are averaged over the whole domain and on time in the quasi steady state regime. The coarse grid results are averaged over the cross section 3.4 m above entrance and on time, also in the quasi steady state regime. Just as observed for the cross section profiles of Fig. 2, the volume averaged figures of Tab. 3 also show great discrepancies of both the simulations to each other, and to experiment. It is clear that the lack of suitable sub-grid models jeopardizes the coarse grid predictions. Otherwise, the discrepancies of the sub-grid predictions appear much more complex. A downward average solid mass flux is found in contrast to the upward average flux found in the experiment. It is clear that a new gravity compensation must be found so that this parameter comes to become more realistic. The solid phase

viscosity resulted two orders of magnitude lower than the experimental figure. A solid phase restitution coefficient of 0.9 was enforced, which was found adequate for getting a correct flow topology. A restitution coefficient of 0.9999999 would be required for the solid phase viscosity to match the order of magnitude of the experimental 0.509 Ns/m^2. In this case, however, the collisions among particles become virtually elastic, and the flow topology results free of clusters. Therefore, imposing a realistic solid phase viscosity produces an unreal flow topology. It becomes clear that better kinetic theory based correlations are required, and that the theory itself needs to be improved.

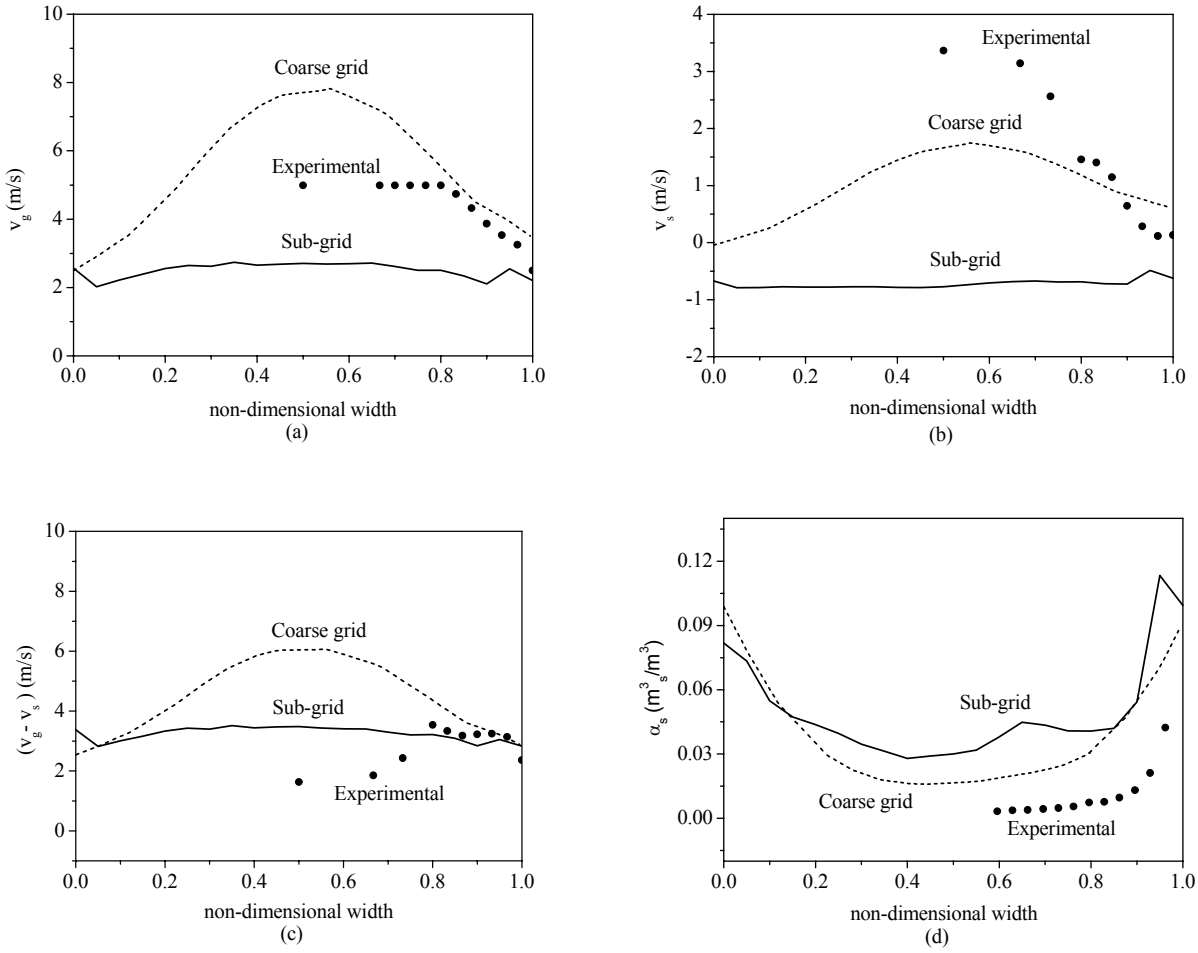


Figure 2. Time averaged profiles of gas axial velocity (a), solid axial velocity (b), slip velocity (c), and solid volume fraction (d), over a central line through the cross section of the domain at 4 cm above entrance for the sub-grid simulation, and at 3.4 m above entrance for the experimental data of Luo (1987) (•) and for the coarse grid simulation (Milioli, 2006).

Table 3. Averaged parameters for the sub-grid and coarse grid simulations, and experimental.

		Sub-grid (*)	Coarse grid (**) (Milioli, 2006)	Experimental (Luo, 1987)
M_s (†)	(kg/m^{2}s)	- 84.8	46.5	27.2
μ_s	(Ns/m^2)	0.00836	0.509	0.509
$v_g - v_s$	(m/s)	3.14	4.58	2.54

(*) Averaged over the domain and on time in the quasi steady state regime; (**) Averaged over the cross section 3.4 m above entrance and on time in the quasi steady state regime;
(†) M_s - solid mass flux.

5. CONCLUSIONS

Two-fluid modeling was applied to simulate a typical riser flow. Predictions of a sub-grid simulation were presented in comparison to the coarse grid simulation of Milioli (2006), and in comparison to experiment. It was shown that none of the simulations correctly predicted experiment. Clearly, the lack of suitable sub-grid models jeopardizes the coarse grid predictions. Regarding the sub-grid simulation, it became clear that a new gravity compensation must be found so that realistic solid mass fluxes can be found. It was observed that applying a solid phase restitution coefficient that gives rise to a realistic solid phase viscosity virtually destroys the flow topology. This suggests that better kinetic theory based correlations are required, and that the theory itself needs improvement.

6. ACKNOWLEDGEMENTS

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