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TWO-FLUID SIMULATION OF THE GAS-SOLID FLOW IN THE RISER OF A CIRCULATING FLUIDIZED BED

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Abstract.*The complex gas-solid flow patterns that develop inside risers of circulating fluidized bed reactors determine reaction rates, so that rigorous hydrodynamic descriptions are required. Two-fluid modeling is currently considered to be the most practical choice for providing such descriptions. However, while producing qualitatively correct results, current two fluid models are still very crude and quantitative accuracy seem to be out of reach. This work brings a discussion relevant to this issue. A a two-fluid simulation is performed to describe the hydrodynamics of a riser flow. Operational conditions typical of circulating fluidized bed coal combustion are considered. Time averaged results are produced and compared to both experiment and other literature two-fluid predictions. A discussion is provided regarding the accuracy of the results. It is concluded that the current two-fluid models applied to gas-solid flows are still very crude, and can not provide quantitative accurate results.*

Keywords*. two-fluid model; two-fluid simulation; circulating fluidized bed; gas-solid flow.*

1. Introduction

Gas-solid flows in risers of circulating fluidized beds are characterized by highly intense formation and dissipation of coherent structures generally known as clusters. The chaotic motion of clusters cause the hydrodynamics to be quite unstable and turbulent. Clusters are formed due to inelastic collisions among particles. Yet, those collisions are supposed to be significantly affected by the interstitial gas phase, which acts on the particles causing both velocity fluctuations and dumping. These effects are also responsible for cluster dissipation.

Any mathematical model for accurately predicting reaction yields in risers must include accurate hydrodynamic descriptions. Currently, the most practical approach for providing such descriptions comes from two-fluid models (Sundaresan, 2000). Such models are based on continuum conservative formulations for all the phases, no matter macroscopically continuous or dispersed (Jackson, 1963; Murray, 1965; Pigford and Barron, 1965; Soo, 1967; Anderson and Jackson, 1967; Drew, 1971).

The main difficulties in two-fluid formulations relate to the establishment of suitable closure relations. Those comprise continuum properties for dispersed phases and parameters defining interface momentum exchanges. Aiming to perform direct simulation alike predictions, micro-scale relations have been derived through an analogy with the kinetic theory of dense gases, known as kinetic theory of granular flows (Jenkins and Savage, 1983; Lun et al., 1984; Gidaspow, 1994). Otherwise, targeting large eddy simulation alike predictions, attempts have been made to correlate meso-scale effects from both empiricism (Miller and Gidaspow, 1992; Huilin and Gidaspow, 2003) and computational experiment (Agrawal et al., 2001; Andrews IV et al., 2005).

Both direct and large eddy simulation alike predictions have been performed by many researchers (Tsuo and Gidaspow, 1990; Mathiesen et al., 2000; Zhang and Van der Hyden, 2001; Agrawal et al., 2001; Cabezas-Gómez and Milioli, 2003; Andrews IV et al., 2005; Georg, 2005; Milioli and Milioli, 2005; among others). Jackson (2000) notes that current two-fluid models seem to catch the right qualitative features of gas-solid flows, but observes that no evidence is provided that they are quantitatively correct. This statement seems to remain up-to-dated. For instance, closure relations derived from the kinetic theory of granular flows have been revised by Boemer et al. (1995) and Van Wachem et al. (1999). In both of those works the authors found very significant divergences among different correlations for the same parameter, indicating that the kinetic theory of granular flows requires improvement.

The lack of knowledge on gas-solid flows turbulence is also an obstacle to overcome in the search for better quantitative results. Sinclair and Jackson (1989) observed that the effect of particles on turbulent structures is not known. Working on this issue, Agrawal et al. (2001) showed through computational experiments that the turbulence of the gas phase has little effect over the average gas-solid flow. Regarding the turbulence of the solid phase, the authors found the meso-scale solid phase viscosity to be inversely proportional to the macro-scale strain rate. They observe that this behavior is contrary to that of single-phase turbulent flows, where the meso-scale viscosity is directly proportional to the macro-scale strain rate. Following the proposition of Agrawal et al. (2001), Andrews IV et al. (2005) formulated closure relations derived from computational experiment, which were reputed as first approximations and ad-hoc.

Despite the efforts, the current literature presents no recognized meso-scale turbulence model suitable for gas-solid flows.

There is no doubt that the current two-fluid models can predict macro-scale turbulence. At what accuracy, however, it remains an open question. This work brings a discussion relevant to this issue. A two-fluid simulation is performed for a case previously simulated by other authors. As expected, a comparative analysis of results showed that the predictions are still very crude, and accuracy is presently out of reach.

2. Two-fluid modeling of gas-solid flows

Two-fluid conservative equations are based on the major hypotheses of continuum and thermodynamic equilibrium commonly applied in fluid mechanics. Two-fluid models for multi-phase flows, including gas-solid flows, are developed from integral mass and momentum balances over suitable control volumes comprising all the phases (see, for instance, Anderson and Jackson, 1967, Ishii, 1975, Gidaspow, 1994, Enwald et al., 1996). The theorems of Leibniz and Gauss are applied to the integral balances giving rise to local instantaneous conservative equations for each phase and jump conditions describing interface interactions among phases. Then, averaging procedures are applied for providing averaged equations. The interfaces among phases in multi-phase dispersed flows like the gas-solid fluidized flow are defined around a huge number of particles, and are highly dynamical and chaotic. Because of that, local instantaneous eventual formulations become inapplicable. The averaging procedures are used to go around such difficulty. Different averaging procedures may be applied like volume averaging, time averaging and ensemble or statistical averaging. Those procedures are usually assumed equivalent (ergodicity hypothesis).

Closure laws are required to deal with parameters and coefficients present in the average conservative equations, and boundary and initial conditions must be set. The closure laws provide correlations and data for viscous stress tensors, viscosities, pressures and drag. All the phases are commonly assumed to be Newtonian-Stokesian fluids. Pressure and viscosities of solid phases are generally accounted for through semi-empirical correlations. 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. Regarding the solid phase viscosities, only the particle to particle attrition and dumping affects are significant, and correlations are generated through simplified momentum balances combined with empirical data. A stationary interface drag force, empirically correlated, accounts for the interface momentum transfer between the gas and the solid phases. Wall boundary conditions for the solid phase are determined considering either no-slip, free slip or partial slip conditions. For the gas phase the conventional no-slip condition is applied.

Following the above, two different formulations have been applied by most of the researchers. In the first, conservative equations are directly generated for each phase. In the second formulation, conservative equations are generated for the gas phase and for the mixture; from those equations, conservative equations are derived for the solid phase. Gidaspow (1994) named those formulations as models A and B, respectively. The formulation of model A, which is used in this work, is showed next.

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:

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

Solid phase momentum:

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

Stress tensor for phase k:

$$\bar{\bar{\tau}}_k = \mu_k\left[\vec{\nabla}\vec{U}_k + (\vec{\nabla}\vec{U}_k)^T\right] + \lambda_k\left(\vec{\nabla}\cdot\vec{U}_k\right)\bar{\bar{I}} \tag{5}$$

where $\mu_k = \text{constant}$, and $\lambda_k = -\frac{2}{3}\mu_k$.

Solid phase pressure:

$$\vec{\nabla}(\alpha_s P_s) = -G\vec{\nabla}\alpha_s + \vec{\nabla}(\alpha_s P_g) \tag{6}$$

where $G = \exp\left[-20(\alpha_g - 0.62)\right]$ (Gidaspow and Ettehadieh, 1983) (7)

Volumetric continuity:

$$\alpha_g + \alpha_s = 1 \tag{8}$$

External body forces per unit mass:

$$\vec{F}_g = \vec{g} \tag{9}$$

$$\vec{F}_s = \frac{\rho_s - \rho_g}{\rho_s}\vec{g} \tag{10}$$

Equations of state:

$$\rho_g = \frac{P_g W_g}{R_u T} \tag{11}$$

$\rho_s = \text{constant}$.

Interface drag (Gidaspow, 1994):

$$\beta = 150\frac{\alpha_s^2\mu_g}{\alpha_g(d_p\phi_s)^2} + 1.75\frac{\rho_g\alpha_s|v_g - v_s|}{(d_p\phi_s)} \quad \text{for } \alpha_s > 0.2 \text{ (Ergun, 1952)} \tag{13}$$

$$\beta = \frac{3}{4}C_{Ds}\frac{\rho_g\alpha_s\alpha_g|v_g - v_s|}{(d_p\phi_s)}\alpha_g^{-2.65} \quad \text{for } \alpha_s \le 0.2 \text{ (Wen and Yu, 1966)} \tag{14}$$

$$\text{where } C_{Ds} = \begin{cases} \dfrac{24}{Re_P}(1 + 0.15\cdot Re_p^{0.687}) & \text{for } Re_p < 1000 \\ 0.44 & \text{for } Re_p \ge 1000 \end{cases} \quad \text{(Rowe, 1961)} \tag{15}$$

$$\text{with } Re_p = \frac{|v_g - v_s| d_p \rho_g \alpha_g}{\mu_g} \tag{16}$$

The symbols in Eqs. (1) to (16) stand for:

C_D - drag coefficient, non-dimensional
d_p - particle diameter, m

$\vec{F}$ - external body force per unit mass, m/s^2
$\vec{g}$ - gravity acceleration, m/s^2
G - particle-particle elasticity modulus, N/m^2
$\overline{\overline{I}}$ - unit tensor
P - pressure, N/m^2
R_u - ideal gas constant, kJ/kmolK
Re_p - Reynolds number, non-dimensional
t - time, s
T - temperature, K
$\vec{U}$ - average velocity vector, m/s
u, v, w - velocity components at x, y, z directions, m/s

Greek

α - volume fraction, m_k^3/m^3
β - gas-solid friction coefficient, kg/m^3s
λ - bulk viscosity, Ns/m^2
μ - dynamic viscosity, Ns/m^2
ρ - density, kg/m^3
$\overline{\overline{\tau}}$ - viscous stress tensor, N/m^2
ϕ - particle sphereicity, 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 CFX5.7 (CFX5.7, 2004 a, b, c) is used. An element-based finite volume discretization method is followed. Non-structured meshes are applied in Cartesian coordinate system. Tetrahedral 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 are 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. Simulation

Risers can not operate in real steady state conditions. Instead, they operate in pseudo-permanent or statistically steady state flow regimes, imposing numerical simulations to be transient. From a given initial condition, a simulation goes through an early stage, and finally reaches the so called statistically steady state regime. For practical purposes, this regime is considered to be reached when all the flow parameters start to oscillate around well defined averages.

The early transient stage is not of higher interest, so that this step is here simulated applying a distorted time numerical advance. Of course, the distorted time advance is not expected to lead to any convergence since the flow never reaches a true steady state regime. However, the iterative marching on distorted time allows to quickly overcome the early stage, and a real time advance simulation may be engaged. When the simulation is switched from distorted time to real time advance, converged predictions are found which are supposed to be generated directly inside the statistically steady state regime. A discussion on that matter can be found in Milioli and Milioli (2005).

In the present simulation 10 seconds of real fluidization were generated inside the statistically steady state regime, taking about 240 days of wall clock processing in a cluster of PCs with 20 processors Intel Xeon 3.06 MHz.

The hydrodynamic conditions assumed in the present simulation have already been considered by other authors, and are typical of circulating fluidized bed coal combustion. The solid mass flux of 24.9 kg/m^2s, particulate size of 520 μm, and the reactor size (height of 5.56 m and width of 7.62 cm) were taken from Tsuo (1989). Figure 1 shows the three-dimensional cylindrical geometry that was assumed, and a sample of the numerical mesh. Table 1 brings fluid and particulate properties, initial and boundary conditions, and numerical settings.

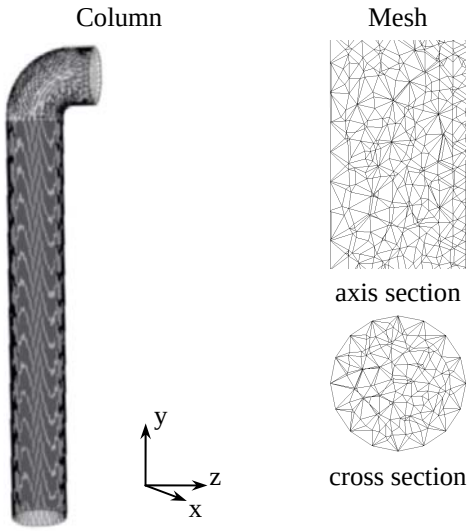


Figure 1. Geometry and a sample of the tetrahedral numerical mesh.

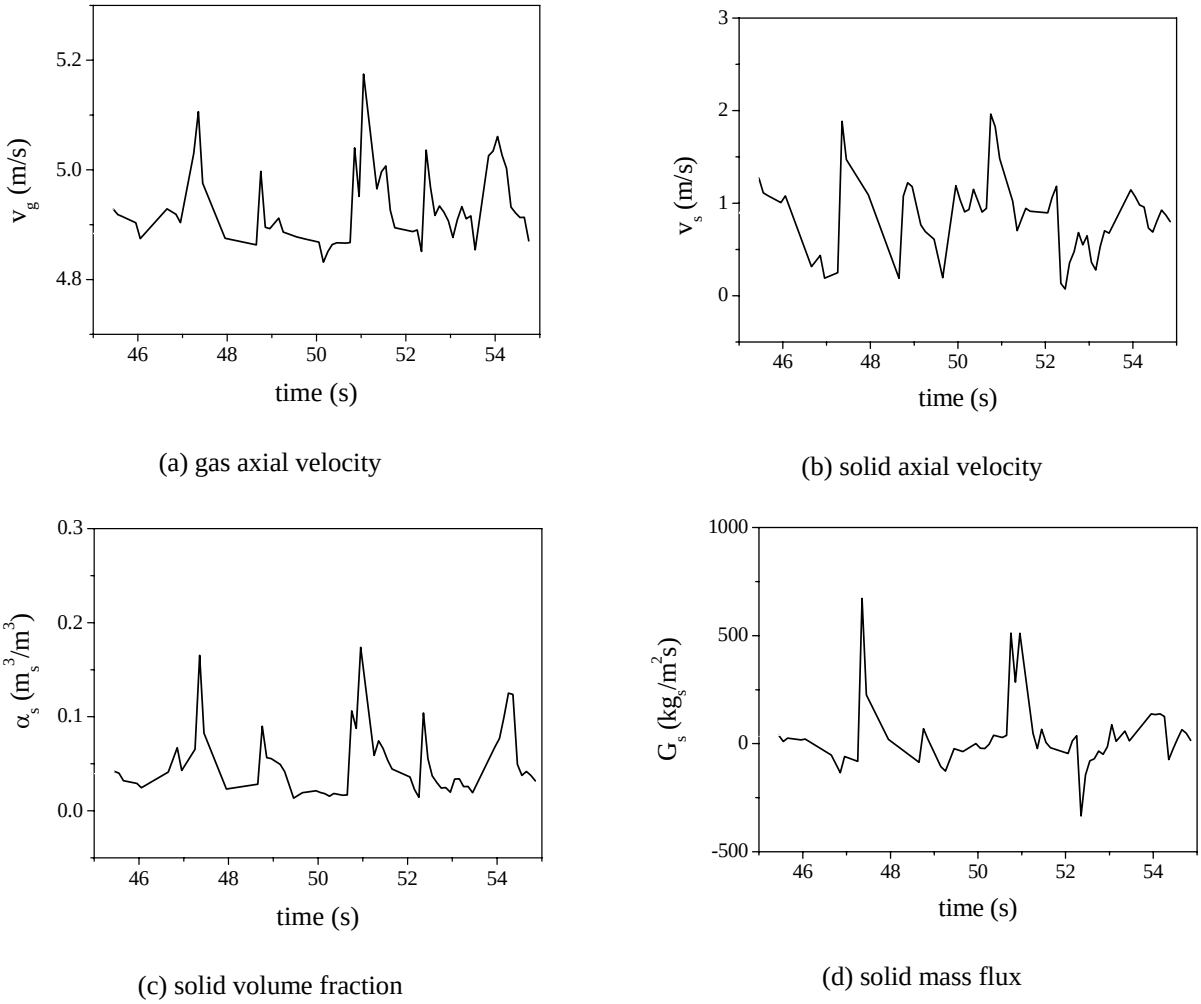
Table 1. Properties, initial and boundary conditions, and numerical settings.

Column	
Diameter = 7.62 cm	Height = 5.56 m
Particulate size = 520 μm	
Solid mass flux (G_s) = 24.9 kg_s/m^2s	
Phases	
g = air at 300 K	s = glass beads at 300 K
Properties	
$\rho_g = 1.1614$ kg/m^3	$\rho_s = 2620$ kg/m^3
$\mu_g = 1.82 \times 10^{-5}$ N/m^{2}s	$\mu_s = 0.509$ N/m^{2}s
$W_g = 28.97$ kg/kmol	$W_s = 60$ kg/kmol
Boundary conditions	
Inlet	
$u_g = 0$ m/s	$u_s = 0$ m/s
$v_g = 4.979$ m/s	$v_s = 0.386$ m/s
$w_g = 0$ m/s	$w_s = 0$ m/s
$\alpha_g = 0.9754$ m_g^3/m^3	$\alpha_s = 0.0246$ m_s^3/m^3
Outlet	Walls
Locally parabolic	g = no-slip
$P_g = 15880$ N/m^2	s = free slip
Initial conditions: as in the inlet, except	
$\alpha_g = 0.62$ m_g^3/m^3	$\alpha_s = 0.38$ m_s^3/m^3
Numerical settings	
Mesh	
Tetrahedrals	= 206229
Average edge length	= 9.4 mm
Nodes	= 42029
rms for convergence	= 1×10^{-5}
Distorted time step	= 1×10^{-3} s
Real time step	= 1×10^{-4} s

4. Results and discussion

Luo (1987) has performed experimental measurements in a riser column, and those data have been compared to results of simulation by different researchers. Luo´s empirical data are known to be imprecise, mainly in regions of low concentration of solids far from the walls (Tsuo and Gidaspow, 1990; Gidaspow, 1994). Owing to that, Luo´s data allow reasonable quantitative comparisons only for regions close to the walls. For regions away from the walls the comparisons must be qualitative only. Despite the drawbacks, Luo's are the best set of empirical data currently available in literature for hydrodynamic conditions typical of coal combustion.

In the present work a two-fluid simulation is performed for Luo's conditions, and the predictions are compared to both experimental data and results of other simulations. Time averaged results are considered which were produced for a time interval of 10 seconds of real fluidization inside the statistically steady state regime. Figure (2) shows the transient behavior of the gas and solid axial velocities, solid volume fraction and solid mass flux, averaged over the cross section at 3.4 m above entrance. All the graphs show profiles oscillating around well defined time averages, indicating that the results stand for the statistically steady state regime.



(a) gas axial velocity

(b) solid axial velocity

(c) solid volume fraction

(d) solid mass flux

Figure 2. Transient behavior of parameters averaged over the cross section at 3.4 m above entrance, for a time interval of 10 seconds inside the statistically steady state regime.

The present time averaged results are compared to the time averaged predictions of Tsuo and Gidaspow (1990), Cabezas-Gómez and Mililoli (2003), and Georg (2005). All of those simulations, including that of the present work, were performed for the operational conditions of Luo (1987). All of the simulations applied two-fluid modeling under the conditions stated in Tab. (1). However, there are a number of model and numerical differences. Tsuo and Gidaspow (1990) and Cabezas-Gómez and Milioli (2003) performed simulations in two-dimensional very coarse meshes, using model B, through the code MFIX in former versions. Georg (2005) and the present work applied three-dimensional finer meshes, even though still quite coarse, using model A, through the code CFX. Table (2) shows the main differences implemented in the different simulations, i.e., phases which are treated as continuum, wall boundary condition for the solid phase, domain and numerical mesh, interpolation scheme used in the discretization of advection

terms, and time averaging interval. Besides those features, there are other differences related to initial conditions, exit boundary conditions, numerical methods (treatment of pressure x velocity coupling, solution technique, type of numerical mesh, time advance, convergence criterion), and computers that were used.

Table 2. Main differences implemented in different simulations of Luo's set up.

	Tsuo and Gidaspow (1990)	Cabezas-Gómez and Milioli (2003)	Georg (2005)	Present work
continuum hypothesis	gas phase and mixture (model B)	gas phase and mixture (model B)	gas and solid phases (model A)	gas and solid phases (model A)
solid phase wall boundary condition	partial slip	partial slip	no-slip	free slip
domain and numerical mesh	two-dimensional, rectangular uniform mesh 7.62 x 76.2 mm	two-dimensional, rectangular uniform mesh 7.62 x 76.2 mm	three-dimensional, hexahedrical uniform mesh 5.1 x 5.1 x 9.3 mm	three-dimensional, tetrahedrical non-uniform mesh, 9.4 mm average edge
interpolation scheme for advective terms	1st. order upwind	1st. order upwind	2nd. order high resolution	2nd. order high resolution
time averaging interval	from 10 to 15 s of simulation	from 20 to 100 s of simulation	from 2.84 to 12.84 s of simulation	10 s inside the statistically steady state regime

All of the features considered in Tab. (2) significantly affect predictions. The character two or three-dimensional and the refinement of the numerical mesh, and the advective interpolative scheme, are considered critical features. The time averaging interval also becomes a critical factor if the averaging is not performed inside the statistically steady state regime. The wall boundary condition for the solid phase is expected to considerably affect the predictions only in regions close to the walls. Regarding the application of the continuum hypothesis, this feature is included in Tab. (2) only to emphasize the conceptual differences among the models, since this factor is known not to considerably affect predictions (Agrawal et al., 2001).

Figures (3) to (6) show the time averaged predictions of the present work compared to experimental data and other literature simulations. The figures show profiles through the diameter of the column, in the cross section 3.4 m above entrance, for, respectively, gas and solid axial velocities, solid volume fraction and solid mass flux. Great deviations regarding the empirical data are observed for all the simulations, except that of Tsuo and Gidaspow (1990). This was unexpected since those authors applied very coarse two-dimensional meshes and first order upwind for the advectives, in contrast to the more refined three-dimensional meshes and the second order high resolution scheme for the advectives applied by Georg (2005) and in the present work. This contradiction is an evidence of the roughness of the current two-fluid models.

As seen in Figs. (3) and (4), the present simulation predicts higher axial velocities at the walls for both phases in comparison to the other simulations. Figure (5) shows that the solid volume fractions of the present simulation are also higher, and even higher close to the walls. Those effects are possibly due to the application, in the present simulation. of free slip for the solid at the walls, while the other simulations applied either partial or non-slip conditions.

Figure (4) shows that the average solid axial velocity predicted in the present simulation resulted positive close to the walls. In spite of that, very high downward solid mass fluxes were observed in these regions, as seen in Fig. (6). The above is no contradiction, meaning only that negative solid axial velocities occur accompanied of high solid concentrations, while positive velocities occur accompanied of lower solid concentrations.

Figure (6) clearly shows that the results of Cabezas-Gómez and Milioli (2003), Georg (2005) and the present predictions are similar, and are considerably deviated from the empirical data of Luo (1987). Otherwise, the predictions of Tsuo and Gidaspow (1990) are very close to experiment. Table (3) shows the solid mass fluxes averaged both on time and through the diameter of the column, for the various simulations and empirical. A solid mass flux of 24.9 kg/m^2s is imposed at the bottom of the column as an inlet boundary condition. Once the statistically steady state regime is reached, this shall be the time averaged value for any section of the column whether in the experiment or in any of the simulations. Note that the empirical data of Luo (1987) provided the correct solid mass flux with good approximation. This shows that the empirical profiles of Luo, even though considered imprecise, do provide correct averaged values. Among the simulations, all of them provided very deviated averaged solid mass fluxes, with the exception of the simulation of Tsuo and Gidaspow (1990). There is no plausible explanation for the surprisingly better prediction obtained by those authors. This conclusion is mainly supported on the fact that the simulation of Tsuo and Gidaspow (1990) is identical to that of Cabezas-Gómez and Milioli (2003), being the only difference the averaging time interval. While Tsuo and Gidaspow (1990) averaged over an interval of 5 seconds, Cabezas-Gómez and Milioli averaged over an

interval of 80 seconds. It was expected that the results of Cabezas-Gómez and Milioli (2003) were better than those of Tsuo and Gidaspow (1990) since a more representative averaging time interval was considered.

In this work, contrary to the expected, an averaged solid mass flux was found which was no better than those predicted by the other simulations. In comparison to Cabezas-Gómez and Milioli (2003), the expectation was justified by the use of a three-dimensional more refined mesh, and the application of a second order interpolation scheme for the advection terms. Cabezas-Gómez and Milioli (2003) applied a very coarse two-dimensional mesh, and first order upwind on the advectives. In comparison to Georg (2005), the expectation was justified since the present time averaging was performed entirely inside the statistically steady state regime. Georg (2005) considered an averaging time interval only partially inside the statistically steady state regime. Those facts once more evidence the crudeness of the current two-fluid models applied to gas-solid flows.

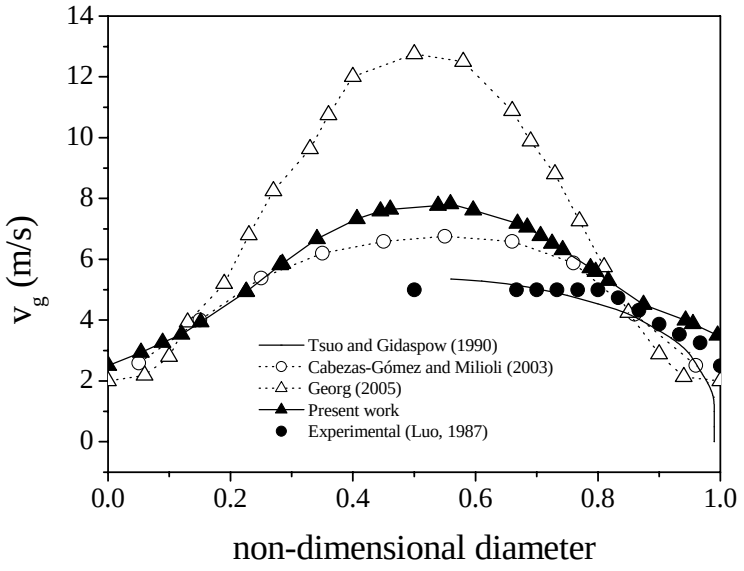


Figure 3. Time averaged profiles of gas axial velocity through the diameter of the column, in the cross section 3.4 m above entrance.

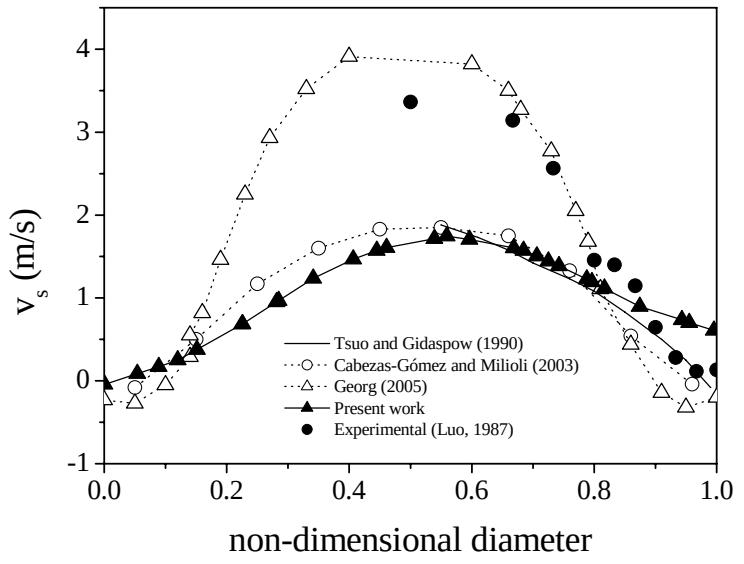


Figure 4. Time averaged profiles of solid axial velocity through the diameter of the column, in the cross section 3.4 m above entrance.

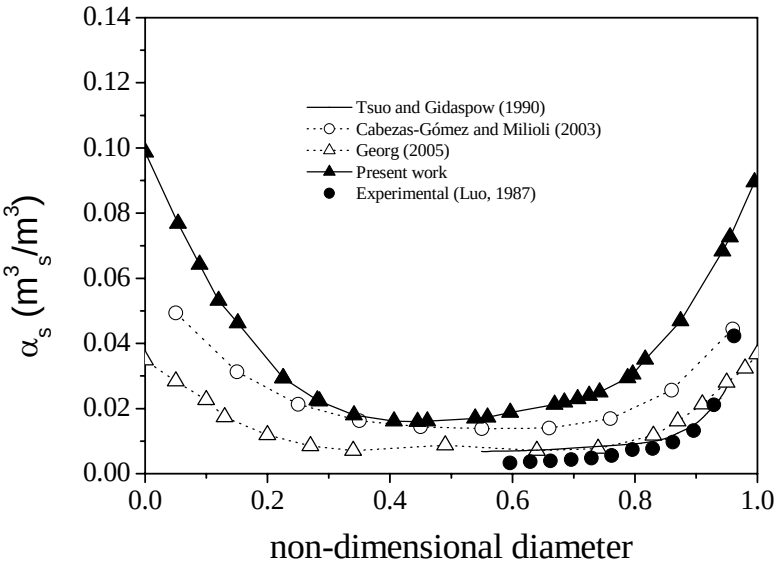


Figure 5. Time averaged profiles of solid volume fraction through the diameter of the column, in the cross section 3.4 m above entrance.

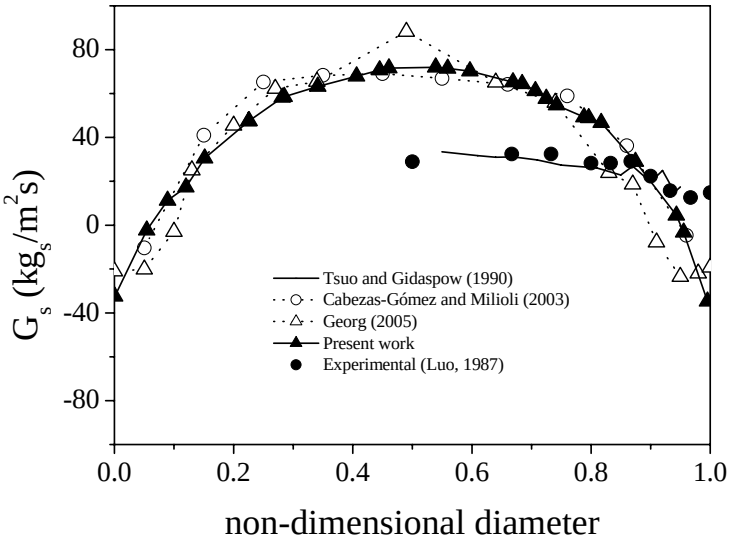


Figure 6. Time averaged profiles of solid mass flux through the diameter of the column, in the cross section 3.4 m above entrance.

Table 3. Solid mass fluxes averaged both on time and through the diameter of the column, from the profiles of Fig. (6), for the various simulations and empirical.

Present work	Georg (2005)	Cabezas-Gómez and Milioli (2003)	Tsuo and Gidaspow (1990) *	Luo (1987) (empírical) *
43.4	41.6	46.5	24.5	27.2

* symmetry was assumed.

5. Conclusions

A two-fluid simulation was performed for the gas-solid flow in the riser of a circulating fluidized bed. A total of 10 seconds or real fluidization were provided. Cross section averaged results were produced showing that the predictions were performed entirely inside the statistically steady state regime.

Time averaged results were derived and compared to both empirical data and predictions from other literature two-fluid simulations. Great quantitative differences were observed among the results of different simulations, and from those to experiment. A contradiction was observed since the rougher of the simulations provided the best of the results. Also, predictions were not improved as expected when a more refined set of conditions were imposed. Those facts support literature observations on the crudeness of the current two-fluid models applied to gas-solid flows. Clearly, in this field, quantitative accuracy is still out of reach.

6. Acknowledgement

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