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MODELLING OF GAS-SOLID FLOWS IN FCC RISER REACTORS: FULLY DEVELOPED FLOW

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ABSTRACT
A two-fluid framework is used with the kinetic theory of granular flows to simulate fully developed gas-solid flows in vertical risers. The computational model was used to simulate the available experimental data over a wide range of operating and design parameters. In addition, several numerical experiments were carried out to understand the influence of riser diameter, particle size, gas and solid flux, solids and gas density on the simulated flow characteristics. The presented results and analysis will be useful for further development of modeling of gas-solid flows in riser reactors.

NOMENCLATURE
C_D	:	Particle drag coefficient
d_p	:	Diameter of particle, m
D	:	Diameter of riser, m
e_p	:	Particle-particle restitution coefficient
G_g	:	Gas flux, kg/m^2 s
G_s	:	Solids flux, kg/m^2 s
k	:	Turbulent kinetic energy, m^2/s^2
Re_p	:	Particle Reynolds number
U_g	:	Axial velocity of gas, m/s
U_s	:	Axial velocity of solid, m/s
U_{sl}	:	Slip velocity of solid, m/s
ϕ	:	Speculiarity coefficient
ε	:	Turbulent energy dissipation rate, m^2/s^3
θ	:	Granular temperature, m^2/s^2
ρ_g	:	Density of gas, kg/m^3
ρ_s	:	Density of solid, kg/m^3

INTRODUCTION
Fluid catalytic cracking (FCC), is one of the most important process in refineries around the world. The cracking of oil is carried out in a short-contact-time riser reactor. Evolutionary design changes are constantly introduced in all components of FCC hardware to enhance the performance (see for example, Johnson et al., 1990). In recent years, computational fluid dynamics is being used to understand the fluid dynamics of FCC system and to evaluate alternative hardware configurations (See for example, Theologos et al., 1997; Ranade, 1998). Emphasis of these studies was on developing a overall reactor (or regenerator) model. Attempt was not made to validate the detailed features of predicted gas-solid fluid dynamics.

Several attempts have been made to model gas-solid flows in vertical pipes (Dasgupta et al., 1998; Kuipers and van Swaaij, 1999; Gao et al., 1999). These efforts can be classified into models based on kinetic theory of granular flows (KTGF) and those do not use KTGF. Though recent results, reported by Gao et al. (1999), which show reasonably good agreement with two experimental data sets, were obtained with the model without using KTGF, the models based on KTGF will have much wider applicability. The models based on KTGF will require less ad-hoc adjustments. In this work, we have therefore considered a KTGF based model.

The KTGF was first used by Sinclair and Jackson (1989) to simulate gas-solid flows in risers. Their model was found to exhibit extreme sensitivity with respect to the value of restitution coefficient, e_p. Nieuwland et al. (1996) also observed such an extreme sensitivity. Bolio et al. (1995) reported that such extreme sensitivity could be overcome by including a gas phase turbulence model. Despite these studies, there are no systematic guidelines available to make appropriate selection of models and model parameters (like laminar versus turbulent, values of restitution coefficients and specularity coefficient, inter-phase drag coefficients) for simulating gas-solid flow in industrial risers.

For most of the available studies, the range of gas and solid fluxes investigated is not directly relevant for the operating range of FCC riser reactors. Influence of riser diameter, particle size and density, solids flux on various flow characteristics (pressure drop, solid volume fraction profiles and so on) has not been studied systematically. In this work, we have computationally investigated fully developed gas-solid flows in risers to address some of these issues. The computational model was first validated by comparing predicted results with experimental data obtained at relatively low solid flux. It was then used to simulate experimental data at higher solid flux. However, most of such experimental data is available only for the small diameter risers. Instead of attempting to fit the model parameters to describe these data, several numerical experiments were carried out to understand influence of riser diameter, particle diameter, solids flux etc. on characteristics of gas-solid flux. The results of these numerical experiments were analyzed with reference to earlier comparisons to draw some conclusions and suggestions for further research.

COMPUTATIONAL MODEL

In this work, we have used a model proposed by Sinclair and coworkers (Sinclair and Jackson, 1989; Bolio et al., 1995). In this model, a two-fluid framework is used with the kinetic theory of granular flows to formulate the governing transport equations for gas-solid flows. Initially gas-solid flow in a vertical riser was simulated by considering a two- dimensional axis-symmetric geometry, with the entire riser height to ensure fully developed flow near the outlet. For such a case, the simulated flow near the outlet will be more or less independent of the inlet boundary conditions. The fully developed flow can also be simulated by considering a very short riser with periodic (translationally) boundaries. Considering the substantial reduction in computational resource for such case, most of the simulations were carried out for such configuration. The model was mapped on to a commercial CFD code, FLUENT version 4.5 (of Fluent Inc., USA) with the help of user defined subroutines. A computational grid used in this work is shown in Figure 1.

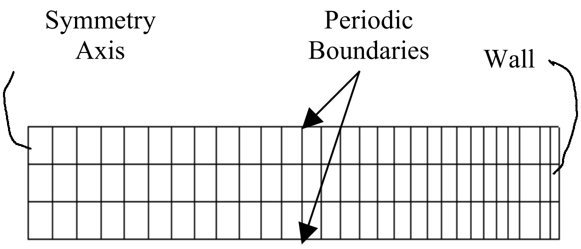

Figure 1: Computational Grid

For each simulation, superficial gas and solid velocities were specified. Computations were started by setting the initial guess equal to these specified velocities. After each time step (of 0.001 s), all the variables except the fluid pressure at inlet were set from the values calculated at the corresponding outlet computational cells. While setting the gas and solid axial velocity at the inlet, a correction was made to enforce the specified net gas and solid fluxes. At the riser wall, boundary conditions proposed by Sinclair and Jackson (1989) were used for solids axial velocity and granular temperature. For the gas phase, usual no slip boundary conditions (with wall functions) was used.

For estimating the interphase drag force, a correlation proposed by Wen and Yu (1966) was used. For the gas-solid flows considered in this work, the contributions of lift and virtual mass forces were negligible. Kinetic theory of granular flows was used to calculate other relevant properties (such as solids viscosity, pressure). Standard k-ε model was used to simulate gas phase turbulence. In order to consider the solid phase turbulence, the time averaged granular temperature equation was solved. Additional terms like dissipation of solid phase turbulence, correlation between fluctuations of granular temperature and solids phase volume fraction were considered in the model. For the sake of brevity, the governing equations are not listed here. The complete set of governing equations may be obtained by referring to the manuals of Fluent (Fluent 4.5 Update manual, 1998). Using these governing equations and described boundary conditions, transient simulations were carried out until the fully developed steady state results are obtained. These results are discussed in the following section.

RESULTS AND DISCUSSION

Bolio et al. (1995) have reported good agreement between model predictions and experimental data of Tsuiji (1984). Instead of repeating those simulations, in this work, we have simulated gas-solid flow corresponding to experimental conditions of Yang (1991). The value of solid flux used in these experiments was also rather low (10 kg/m^{2}s). The predicted results are compared with the experimental data in Figure 2.

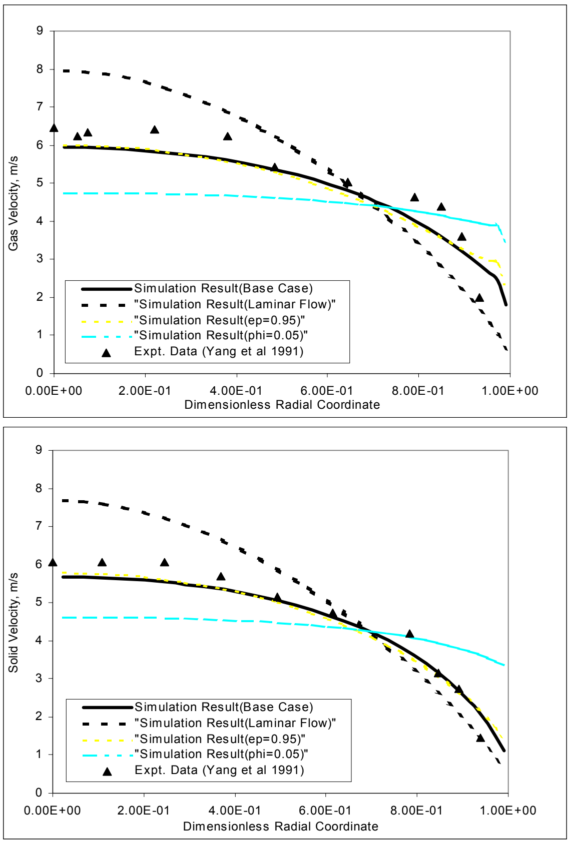

Figure 2: Verification of Model at Low Solid Flux (d_p = 54 μm, ρ_s = 1545 kg/m^3, D = 0.14 m, U_g = 4.33 m/s, G_s = 10 kg/m^{2}s).

Initially, gas-solid flow was simulated without considering the turbulence model. It can be seen that for this case, the predicted centerline gas velocity is significantly higher than that reported by Yang (1991). Predicted results after considering the turbulence model show much better agreement with experimental data (see Figure 2). In order to verify that the predicted results are not unreasonably sensitive to the value of particle-particle restitution coefficient, gas-solid flow simulations were also carried out with restitution coefficient of 0.95. The predicted radial profiles of gas and solid velocity are almost same as those obtained with restitution coefficient of 1.0. The predicted radial profiles of solid hold-up are shown in Figure 3.

It can be seen that lower value of particle-particle restitution coefficient predicts higher value of centerline solid hold-up. Unfortunately, experimental data of solid hold- up is not available. The predicted profiles of granular temperature for the two values of the restitution coefficient also show significant difference at the region near the symmetry axis. Despite these differences, it can be concluded that the model does not exhibit an extreme sensitivity to the value of restitution coefficient. The influence of the value of speculiarity parameter on predicted results was also examined. Kuipers and coworkers have used the value of speculiarity coefficient as 0.5 while Bolio et al. (1995) have used a very small value (of 0.002). The reduction in the value of speculiarity parameter causes more slip at the riser walls leading to flatter profile of solid velocity (see Figure 2). An order of magnitude decrease in the value of speculiarity coefficient (0.05 from 0.5) increased the wall slip of solid particles from 0.9 m/s to 3.2 m/s. It can be seen that the predicted results obtained with the value of 0.5 showed much better agreement with experimental data (Figure 2). Considering these results, for all the subsequent simulations, particle-particle restitution coefficient, particle-wall restitution coefficient and speculiarity coefficients were set to 1.0, 0.9 and 0.5 respectively. With these parameter settings, the computational model was found to give satisfactory agreement with the experimental data of Yang (1991).

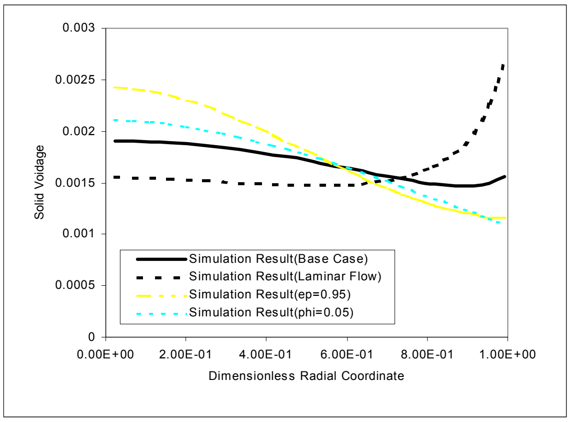

Figure 3: Sensitivity of predicted solid hold-up profiles with model parameters (simulations of experimental conditions of Yang, 1991).

For simulating gas-solid flows in FCC riser, it is necessary to simulate flows at high solid fluxes. At higher solid flux, radial segregation increases and a significant downflow of solids may occur in the near wall region in the riser. Several authors have reported such downflow of solids near the wall (for example, van Bruegel et al., 1969; Bader, 1988; Nieuwland. 1996; Derouin et al. 1997). We simulated experimental conditions reported in these studies using the same computational model, which was used to simulate the data of Yang (1991). The typical comparisons at higher solid fluxes are shown in Figures 4.

It can be seen that the agreement between predicted results and experimental data has significantly deteriorated and the model used in the present work has failed to capture the significant downflow near the riser wall. It was interesting to note that the simulations showed the downflow at the wall if the simulations were carried out without considering the gas phase turbulence model. Results for such a case predict a much larger center line solids velocity than observed experimentally (Figure 4). The results of Pita and Sundersan (1991) and Yasuna et al. (1995) showed good agreement between predicted results and experimental data of Bader et al. (1988) without including the turbulence model. Their computational model, however, exhibits an extreme sensitivity with respect to particle-particle restitution coefficient. It therefore can not be used for simulating practical riser flows. Recently Kuipers and van Swaaij (1999) also observed that it was not possible to simulate the downflow near the riser wall without modifying the underlying model.

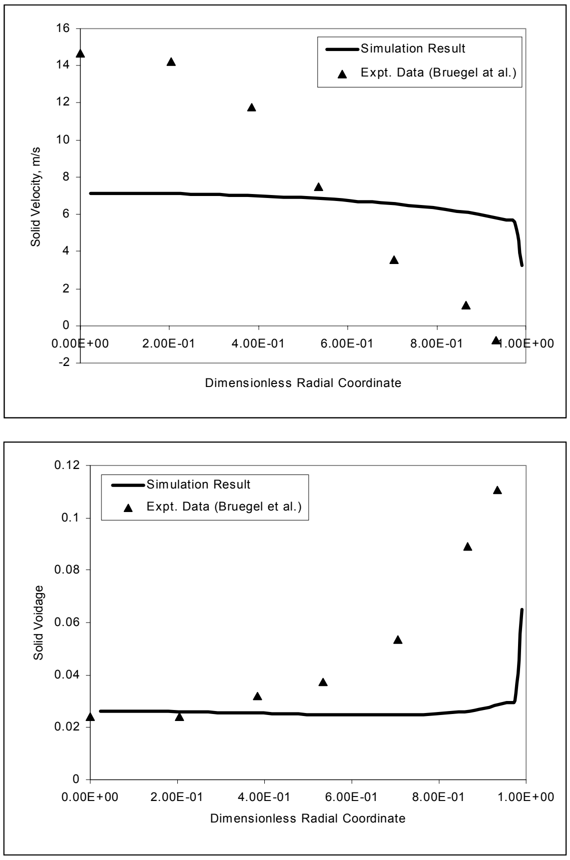

Figure 4: Comparison with experimental data of van Bruegel et al., 1969 (d_p = 40 μm, ρ_s = 2300 kg/m^3, D = 0.30 m, U_g = 6.30 m/s, G_s = 390 kg/m^{2}s).

The pronounced lateral segregation and solids downflow near the wall with velocities much higher than terminal-settling velocities may occur due to the formation of clusters. When such clusters form, the typical size of the cluster and how these clusters affect the dynamics of gas-solid flows in vertical risers has not been properly understood. Several ad-hoc modifications based on fitting the limited set of experimental data have been attempted. Matsen (1982) has proposed a correlation for estimating slip velocity of clusters as a function of single particle terminal settling velocity and volume fraction of solids. The ratio of slip velocity to terminal settling velocity at 10

% solids volume fraction is about 5. Kuipers and van Swaaij (1999) have used a correlation proposed by Nieuland et al. (1994) to correct the interphase drag coefficient to account for cluster formation in the riser flows. This correlation predicts the ratio of slip velocity to terminal settling velocity as about 30. Thus, these two correlations for accounting the influence of clusters on interphase drag force term differ significantly from each other. It appears that the cluster formation, their size and slip velocity may be function of more parameters than just the solids volume fraction and terminal settling velocity. Without generating such information through further research, it will not be beneficial to incorporate empirical corrections to the interphase drag force term in the model.

In addition to the drag correction, it may be possible to get better agreement between simulated results and experimental data by adjusting the values of model parameters. Instead of employing such ad-hoc adjustments to get the better fit, in the present work, numerical experiments were carried out with the basic model to examine influence of relevant variables like riser diameter, particle diameter, solid flux on predicted results. The results of these numerical experiments are discussed in light of comparison of predicted results with the reported experimental data listed above, with an intention of identifying issues requiring further research.

For carrying out numerical experiments, a base case of gas-solid flow was considered for particle diameter of 100 μm, particle density of 2000 kg/m^3, gas density of 5 kg/m^3, riser diameter of 0.30 m, gas superficial velocity of 10 m/s and solid flux of 400 kg/m^{2}s. The model discussed before was used along with the turbulence model to simulate the base case and various other cases with systematic variation of the main governing parameters of gas-solid flows in risers. The data used for these numerical experiments are listed in Table 1. Additional simulations were also carried out to examine interaction between various parameters by simultaneously varying more than one parameter. Unless otherwise mentioned, for all the simulations, particle-particle restitution coefficient was set to one, particle-wall restitution coefficient was set to 0.9 and speculiarity coefficient was set to 0.5. Influence of various parameters on predicted values of solid velocity, slip velocity, solid volume fraction, solids granular temperature and gas phase turbulent kinetic energy was studied

Influence of Riser Diameter: The predicted results for three different riser diameters are shown in Figure 5. It can be seen that there are significant qualitative differences in the predicted radial profiles for the small diameter riser (0.06 m) and for the larger diameter risers (0.3 and 1.0 m). For the small diameter riser, a pronounced wall peaking was predicted even in absence of cluster corrections. For the large diameter risers, the model predicts qualitatively different profile with minima in solid hold-up near the wall. As the riser diameter increases, the location of maximum in the predicted solid flux profile shifts towards the riser wall. Considering the significant influence of riser diameter on the characteristics of gas-solid flows in risers (especially on solids granular temperature), it will be inappropriate to use the empirical cluster corrections derived by fitting the experimental data obtained in a smaller diameter riser. The formation of clusters and the role of riser diameter in cluster formation need to be studied in detail for developing industrially useful models.

No.	D, m	d_p, μm	ρ_s, kg/m^3	ρ_g, kg/m^3	U_g, m/s	Gs, kg/m^{2}s	Δp/L Pa.m
1	0.30	100	2000	5	10.0	400.	647.17
2	0.06	100	2000	5	10.0	400.	1924.3
3	1.00	100	2000	5	10.0	400.	488.35
4	0.30	200	2000	5	10.0	400.	666.65
5	0.30	050	2000	5	10.0	400.	617.35
6	0.30	100	2000	5	10.0	200.	444.97
7	0.30	100	2000	5	10.0	100.	375.74
8	0.30	100	2000	5	5.0	400	950.21
9	0.30	100	2000	5	5.0	200	528.21
10	0.30	100	1000	5	10.0	400	385.72
11	0.30	100	2000	1	10.0	400	546.67

Table 1: Data Used for Numerical Experiments

Influence of Particle Diameter and Solid Density: Numerical experiments were carried out for three values of particle diameters and two values of solid density. The results are shown in Figure 6.

It can be seen that a smaller particle diameter leads to a flatter profile for solids velocity. As expected, the predicted slip velocity increases with the particle diameter. All the slip velocity profiles exhibit the sharp peak near the riser wall. The predicted solid hold-up profiles for all these fours cases, are not significantly different. The predicted granular temperature increases with particle diameter and particle density, though the shape of the profile remains the same.

Influence of Gas and Solid Flux: Results of the numerical experiments for examining influence of gas and solid flux are shown in Figure 7.

It can be seen that for the same superficial gas velocity, the decrease in solids flux leads to higher granular temperature and higher slip velocities. For the same solids flux, a decrease in gas velocity significantly reduces the granular temperature. Predicted profiles of slip velocity exhibit a maximum in the near wall region, the magnitude of which increases with increasing superficial gas velocity and decreasing solid flux. The computational model however failed to predict any significant downflow of solids even for the highest solids flux (400 kg/m^{2}s) and lowest gas velocity (5 m/s) case. The role of gas phase and secondary solid phase turbulence on radial segregation of solids needs to be studied systematically to evaluate the currently used KTGF based models. The predicted values of pressure drops (see Table 1) show the expected trends. However, unless the downflow near the wall is captured, quantitative comparison with the experimental data will be difficult.

Pita and Sundaresan (1991) have reported results of numerical experiments using their computational model (without including a turbulence model). They have reported the existence of multiplicity for the large diameter risers. In order to examine the possibiilty of multiple solutions, numerical experiments were initiated with several different initial guess fields. However, in none of the case we could detect any multiplicity. The computational model always converged to the same results from any initial guess field. The computational model used in the present work predicted monotonic decrease in pressure drop with increase in riser diameter for the specific values of gas and solid fluxes. This trend is in lline with the observations of Yerushalmi and Avidhan (1985). Pita and Sundaresan's model however predicted a reversal in the trend and subsequent increase in pressure drop with increase in riser diameter beyond certain value of riser diameter (about 0.1 m). Such a reversal in trend may occur if the model predicts the downflow of solids near wall for the large diameter risers. The model used in the present work did not predict any downflow even for the 0.5 m riser. It is necessary to generate systematic data of radial seggregation of solids by conducting experiments at different riser diameters covering the range of particle diameters and gas and solid fluxes relevant for FCC riser flows. The data will also be useful to understand the cluster formation and to quantify their influence on dynamics of gas-solid flows. Since the laminar model was found to predict the downflow near wall at higher solid fluxes, it is necessary to investigate the role of turbulence and interaction of turbulence and solid particles. Instead of empirically adjusting the values of restitution coefficient and speculiarity coefficient, independent measurements of these parameters must accompany the experimental data suggested above. Such experimental work is being initiated using an existing cold flow set-up. Additional numerical experiments are also being carried out to simulate gas-solid flows under idealized situations as limiting cases. An attempt is being made to evolve suitable criteria based on these limiting cases and all the available empirical information, which any computational model should satisfy.

CONCLUSIONS

A two-fluid model was used with the kinetic theory of granular flows to simulate fully developed turbulent gas-solid flows in vertical risers. The computational model was found to give adequate results for simulating dilute gas-solid flows in vertical risers. It however failed to simulate observed downflow of solids at higher values of solid flux. The empirical corrections proposed in the literature differ significantly from each other. In order to understand the behavior of the model, several numerical experiments were carried out to examine influence of riser diameter, particle size, gas and solid flux, solids and gas density on the simulated flow characteristics. These results along with the comparison of experimental data were analyzed to identify crucial issues, which require further research and development to enable adequate simulations of gas-solid flows in a range relevant for FCC riser reactors.

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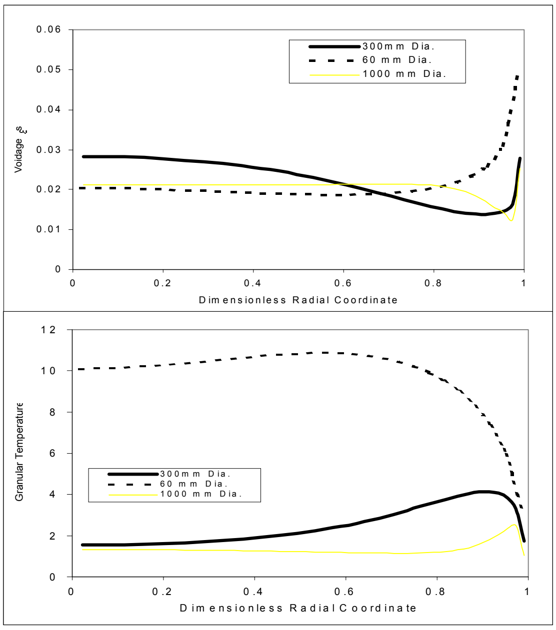

Figure 5: Influence of riser diameter

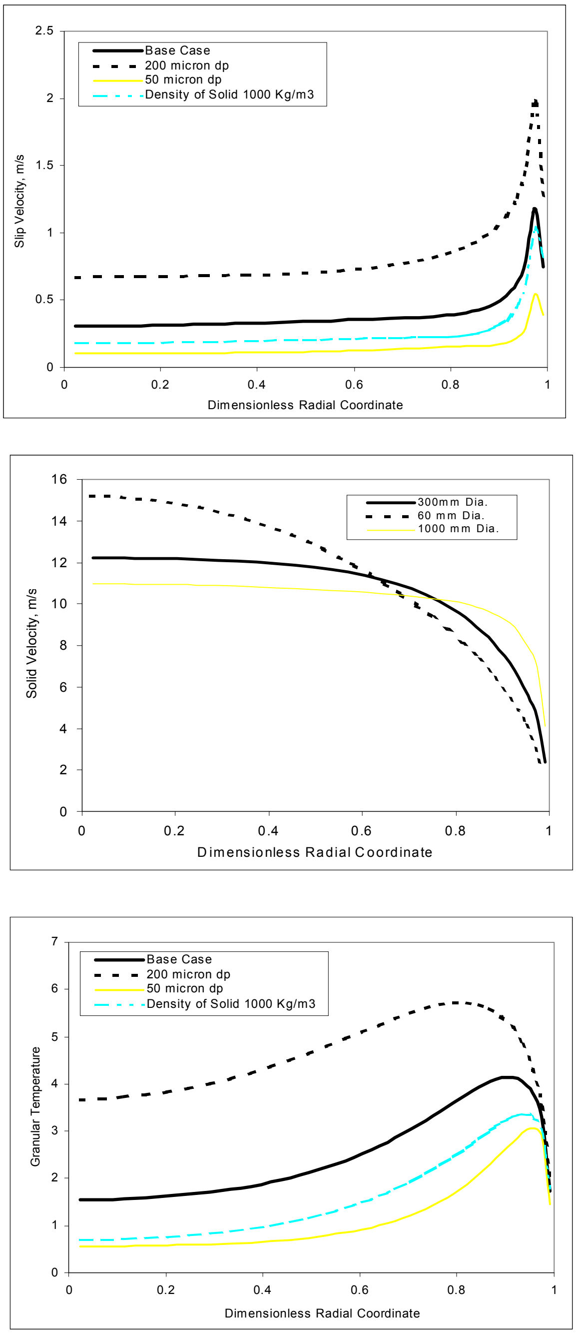

Figure 6: Influence of particle diameter and density

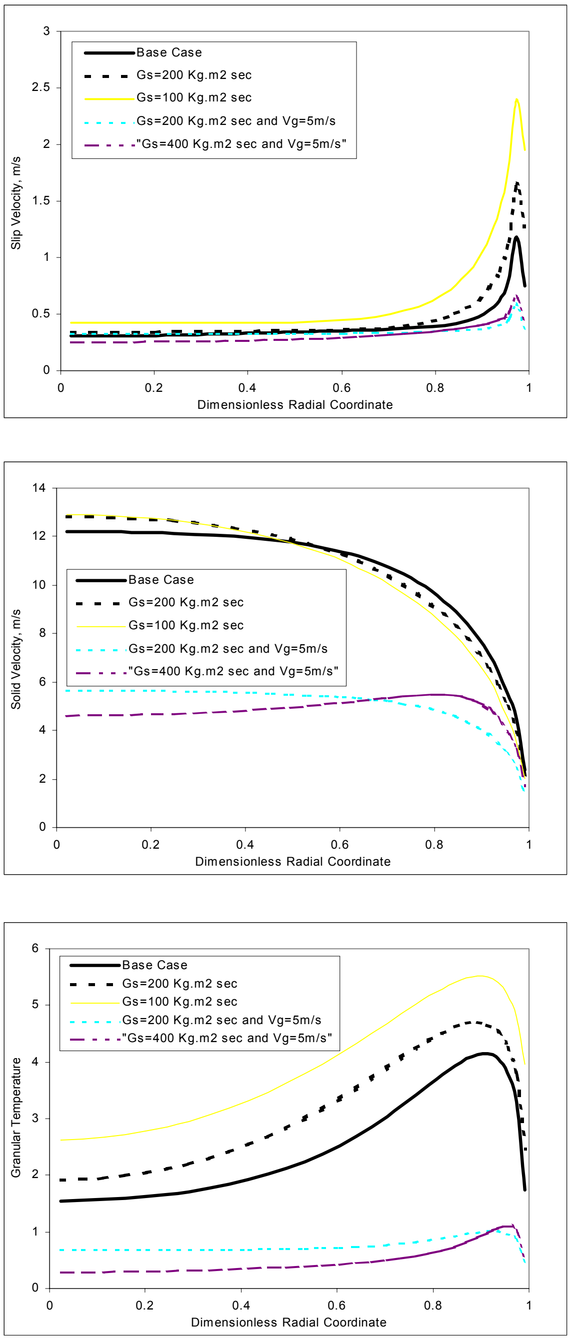

Figure 7: Influence of gas and solid fluxes