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DOE/PC/91297-T4

**DOE/PC/91297-1**

**Quarterly Technical Progress Report**

(March 1, 1994 to May 31, 1994)

**A COMPUTATIONAL MODEL FOR  
COAL TRANSPORT AND COMBUSTION**

**Grant Number: DE-FG22-91PC91297**

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**Submitted to**

**U.S. Department of Energy**

**Pittsburgh Energy Technology Center**

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# **A COMPUTATIONAL MODEL FOR COAL TRANSPORT AND COMBUSTION**

**Grant Number:** DE-FG22-91PC91297

**Project Period:** September 1, 1991 to August 31, 1994

**Contract Recipient:** Clarkson University

**Project Principal Investigator:** Goodarz Ahmadi

**DOE Project Officer:** Dr. Mehrdad Massoudi

## **SUMMARY**

In the period of March 1, 1994 to May 31, 1994, the earlier developed computational models for analyzing flow of granular materials in ducts and passages with bumpy walls were used to analyze Couette and chute flows. The results were compared with the experimental data and good agreement was observed.

Further results on the flows of gas-solid mixtures in vertical ducts were obtained. A computational model for analyzing two-phase flow was developed, and the phasic mean velocity and fluctuation energy profiles were evaluated. The results were compared with the experimental data of Tsuji an co-worker and good agreement was obtained.

Further progress in the experimental study of mono-granular layer simple shear flow device was made. The experimental data concerning the mean granular velocity, fluctuation velocity and solid volume fraction were obtained. The resulting data revealed the importance of fluctuation energy components on dynamics of particulate flows.

## **PROGRESS REPORT**

### **OBJECTIVES**

The objective of this project is to develop an accurate model describing turbulent flows of coal slurries, rapid flows of granular coal-air mixtures, and turbulent coal combustion processes. The other main objective is to develop a computer code incorporating the new model. Experimental verification of the foundation of the model is also included in the study.

### **SIGNIFICANCE TO FOSSIL ENERGY PROGRAM**

A completely satisfactory theory describing the bulk coal transport including the interstitial fluid effects does not exist. This is particularly the case for turbulent flows of dense coal particle-liquid mixtures and chemically active coal combustor flows. Coal slurry and bulk transports, and operation of coal combustors accounts for a substantial portion of the cost of coal energy conversion systems. The major increase in cost arises from the need to over-design these facilities to guarantee reliability. Understanding the flow behavior of relatively dense coal slurries and bulk solids in various geometries including coal combustors, are indispensable to economical design of the needed equipment. This project aims to develop a sound practical model for coal transport and combustion. In addition, a computational predictive capability for analyzing rapid flows of granular coal particles, and reacting and non-reacting turbulent flows of dense or dilute multiphase coal mixtures will be provided.

## HIGHLIGHT OF THE EARLIER ACCOMPLISHMENTS

An experimental setup for generating simple shear flows of a mono-granular layer was constructed. Experimental data for mean velocity, fluctuation energy and solid volume fraction for shearing of 12 mm multi-color glass particles were obtained.

Thermodynamically admissible expressions for the phasic stress tensors, heat and fluctuation energy flux vectors for turbulent multiphase flows were derived. The material parameters of the model were evaluated from the limiting conditions of rapid flows of dry spherical granular particles, and single-phase turbulent fluid flow. The case of simple shear flows of glass beads-water mixtures was studied.

A thermodynamically consistent model for rapid flow of granular materials in a rotating frame of reference, along with a transport equation for the granular kinetic stress tensor were developed. The model parameters for the special case of spherical nearly elastic particles were evaluated. The results for the granular stresses and the normal stress differences were compared with the available simulation data and good agreement was observed.

Effects of frictional loss of energy on rapid granular shear flows were studied. The previously developed kinetic based model was used and the mean velocity, the fluctuation kinetic energy and the solid volume fraction profiles were evaluated under a variety of conditions and different friction coefficients.

A computational model for analyzing rapid granular in complex geometries was developed. The discrete element scheme was used and the granular flow down a chute was analyzed. The results were compared with the experimental data model prediction of Savage, and the existing simulation results, and good agreements were observed. The model was used to analyze granular flows in a duct with an obstructing block.

A computational model for analyzing turbulent two-phase flows with various loadings was developed. The special case of gas-solid flows in a vertical duct was analyzed and the model predictions were favorable compared with the available experimental data.

## COMPUTATIONAL MODEL DEVELOPMENT

The goal of this phase of the study is to develop an appropriate computational scheme for solving granular and two-phase flows.

### Granular Flows with Bumpy Boundary

The boundary condition is known to significantly affect flow and transport of granular materials. Here the effect of bumpy walls with roughnesses comparable to the size of the particle is studied. The kinetic model of granular materials including frictional losses is also used in the analysis. The presence of bumpy boundary conditions leads to a strongly coupled system of governing equations which has to be solved numerically even for the simple case of a Couette flow. As noted in the earlier report, a special discretization scheme for evaluating the granular flow field was developed. The computational model was used and the mean velocity, the fluctuation kinetic energy and the solid volume fraction profiles for granular flows between two parallel walls were evaluated. The results for different values of friction coefficients were presented in the previous report and were compared favorably with the molecular dynamics (MD) simulations of Savage and Dai (1992) for frictionless particles.

Figure 1 presents the mean velocity, the square-root (SR) of fluctuation kinetic energy and the solid volume fraction profiles for different mean concentrations  $v_0$ . In this case, the other parameters are kept fixed with a width to diameter ratio of 10, a coefficient of restitution of  $r=0.7$ , and a coefficient of friction of  $M=0.05$ . As the average solid volume fraction increases, a decrease

in the SR-fluctuation kinetic energy is observed, while the mean velocity profile remains nearly the same.

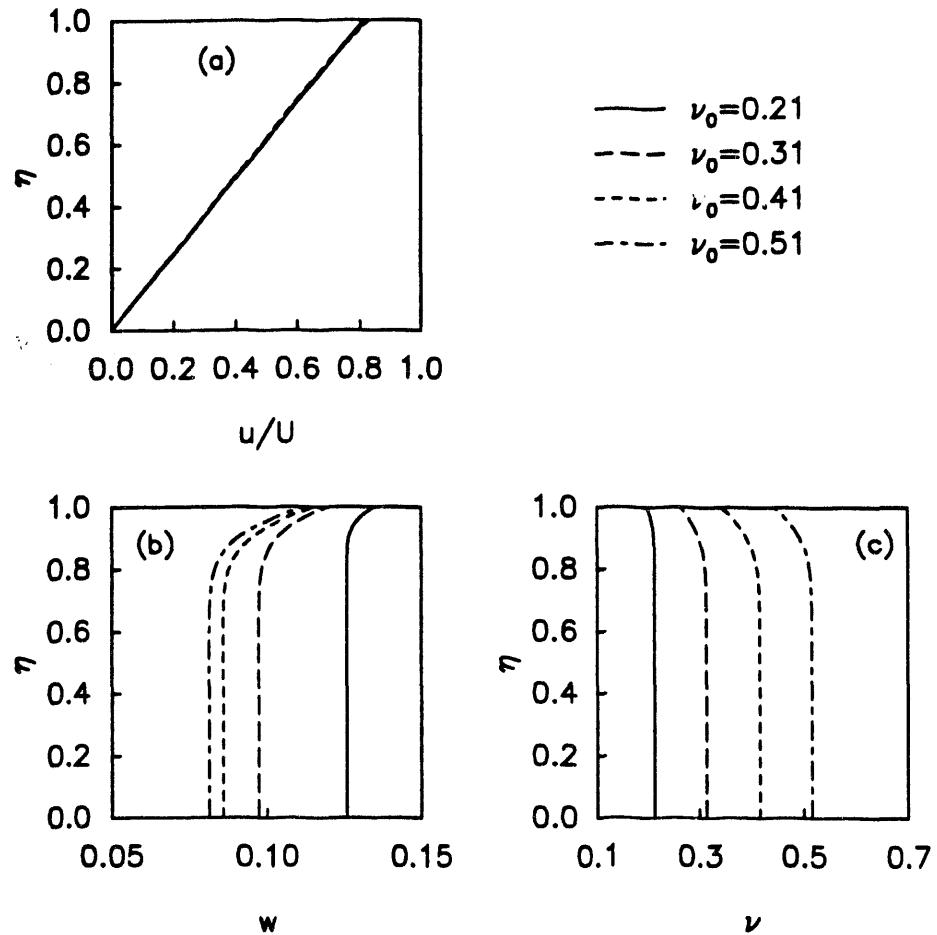


Figure 1. Variations of mean velocity, SR-fluctuation energy and solid volume fraction profiles for different averaged solid volume fractions.

Figure 1a also indicates that the mean velocity profiles for different mean solid volume fractions are roughly linear with slip velocity remaining approximately a constant. The SR-fluctuation kinetic energies are also constant in the mid-region of the duct and increase towards the wall. The concentration profiles show a constant trend in the core region, but decreases toward the bumpy boundary. These results show that the commonly used assumption

that the kinetic energy and the solid volume fraction are constants for Couette flows of granular materials is not quite correct.

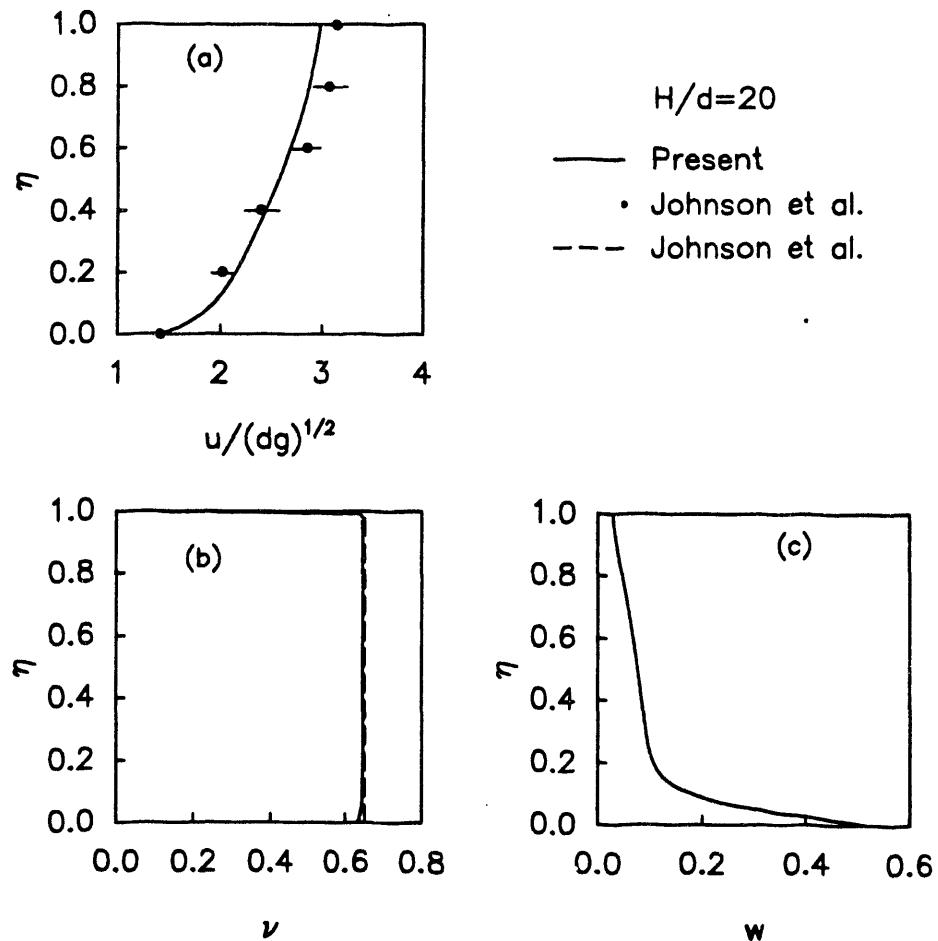


Figure 2. Sample prediction results for granular over a bumpy incline.  
 Comparison with the experimental data of Johnson et al. (1990).

### Granular Gravity Flows

Granular gravity flows over an inclined bumpy chute is an important flow and is often used as a bench mark for test of various theories. The earlier developed kinetic-based model for rapid flows of granular materials which includes the frictional losses of energy during particle-particle and/or particle-wall collisions is used for analyzing granular chute flows. The

predicted mean velocity, fluctuation energy, and solid volume fraction profiles are evaluated and the results are compared with existing experimental data.

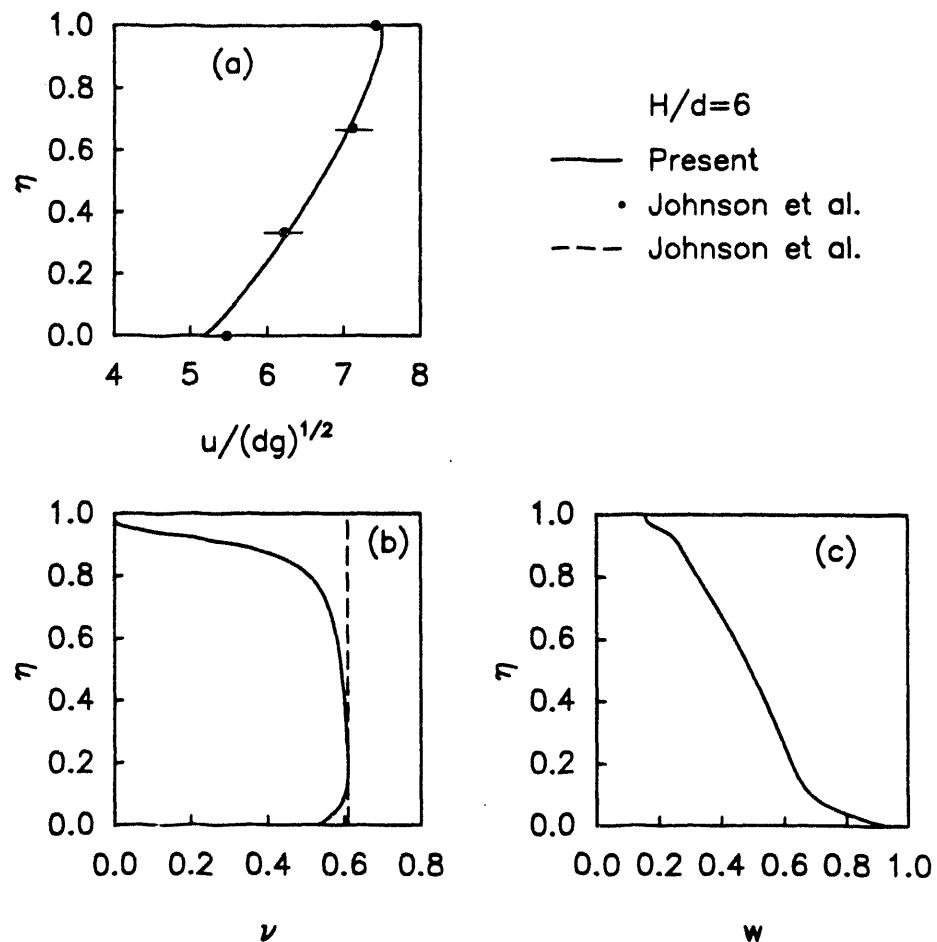


Figure 3. Sample prediction results for granular over a bumpy incline.  
Comparison with the experimental data of Johnson et al. (1990).

Johnson et al. (1990) performed a series of experiments for gravity flow of 1 mm diameter glass beads down an inclined chute with a smooth aluminum plate. The chute was 1.4 m long and 6.35 cm wide, and was bounded by vertical glass walls 12.7 cm high. Their mean velocity data for an inclination angle of  $\alpha=17^\circ$  and  $H/d=20$  are reproduced in figure 2. The present model predictions for the same conditions are also plotted in this figure for comparison.

Here, a coefficient of restitution of  $r=0.91$  and a coefficient of friction of  $\mu=0.45$  for glass beads as suggested by Johnson et al (1990) are used in numerical simulation. The experimental smooth wall surface condition is simulated by considering a wall with closely packed small bumps. Figure 2a shows that the calculated velocity profile is in good agreement with the experimental data. A significant amount of slip at the wall is also noticed in the experiment which is well predicted by the model.

From figure 2b, it is observed that the solid volume fraction remains almost a constant across the chute with a sharp gradient near the free surface. The dashed line in this figure corresponds to the mean solid volume fraction of  $\nu_0=0.65$  reported in the experiment of Johnson et al. (The solid volume fraction and fluctuation kinetic energy profiles were not measured by Johnson et al.). The predicted mean solid volume fraction here is 0.64 which is quite close to the experimental mean solid volume fraction.

Figure 2c shows the variation of SR-fluctuation kinetic energy ( $w$ ) over the incline. It is observed that the SR-fluctuation energy has a large value near the wall and decreases rapidly to about 20% of its wall value at a short distance from the wall. It then decreases gradually toward the free surface. Unfortunately, there is no experimental data for the fluctuation kinetic energy for comparison in this case.

Figure 3 presents the model predictions for  $H/d=6$  and a comparison with the corresponding experimental data of Johnson et al. (1990). The rest of parameters used in this simulation are the same as those of figure 2. Figure 3a shows that the calculated velocity profile is in reasonable agreement with the experimental data. The predicted slip at the wall, however, is slightly lower than that observed in the experiment. This could be due to the bumpy wall boundary model used in the simulation, while the experiment was performed on flat inclined chute. Figure 3b presents the calculated solid volume fraction profile. The dashed line in this

figure corresponds to the experimental mean solid volume fraction. The solid volume fraction remains roughly a constant, except for its rapid decrease in the saltation region, and a decreasing trend in the shearing zone near the wall. The calculated mean solid volume fraction is 0.543, while the experimentally reported value was about 0.61. Figure 3c shows the SR-fluctuation kinetic energy profile. It is observed that  $w$  has a large value near the wall and decrease with the distance from the chute surface.

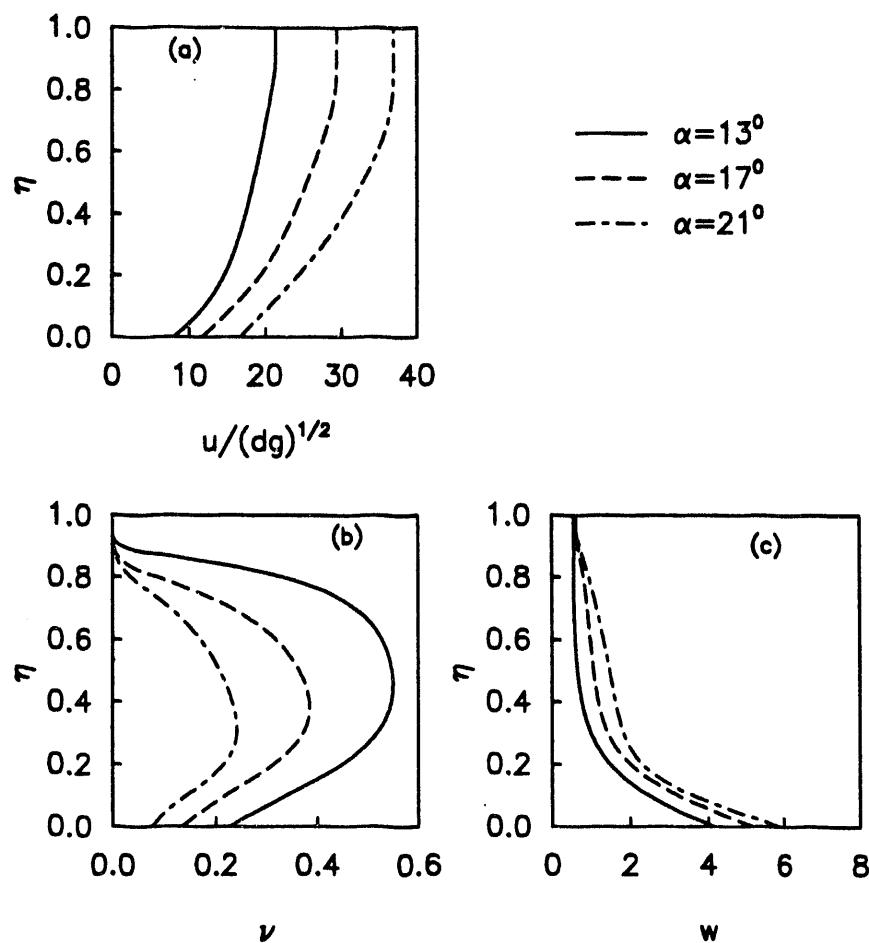


Figure 4. Variation of mean velocity, solid volume fraction and SR-fluctuation energy profiles for granular over a bumpy chute at different inclination angles.

Figure 4 shows variations of velocity, solid volume fraction and SR-fluctuation kinetic

energy profiles for chute inclination angles of  $13^\circ$ ,  $17^\circ$  and  $21^\circ$ . The other parameters are kept fixed at  $r=0.9$ ,  $\mu=0$ , and  $H/d=20$ . The velocity profiles shown in figure 4a indicate that a large slip occurs at the bottom wall. As the inclination angle increases, the mean, as well as the slip velocities increase. Figure 4b shows that the solid volume fraction decreases with increasing  $\alpha$ . The flow is also very sensitive to changes of the inclination angle, since a small change in  $\alpha$  can have a dramatic effect on the flow properties. Saltation regions of very low solid volume fraction near the free surface are also clearly observed. The height of the saltation region increases as the inclination angle increases. Figure 8a also shows that the mean velocity is roughly constant in the saltation region.

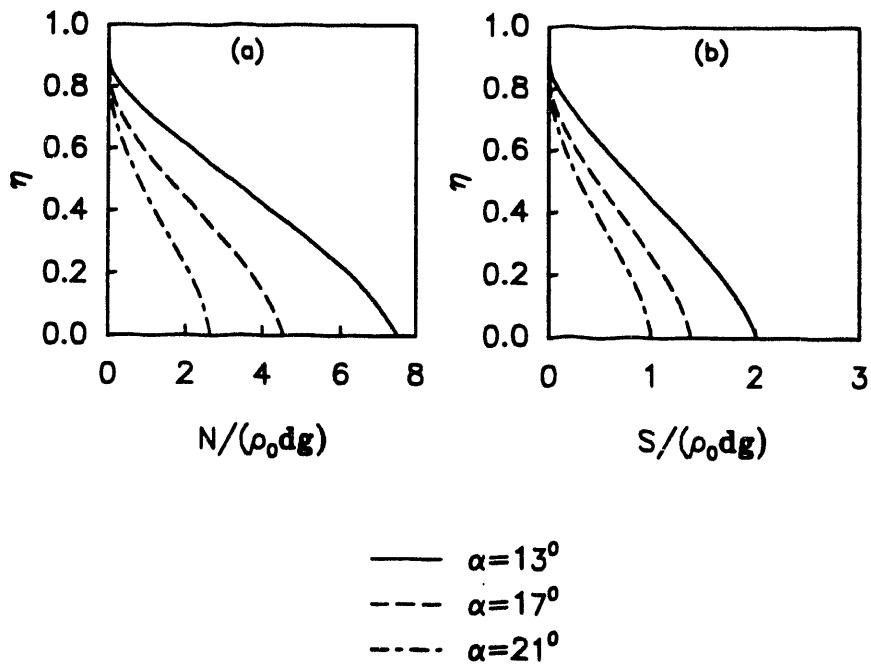


Figure 5. Variation of nondimensional normal and tangential stresses for granular over a bumpy chute at different inclination angles.

Figure 4b shows that the flow maintains a region of low density near the bottom wall, despite the large overburden of material. This phenomenon has been observed experimentally in

chute flows by Bailard (1978) and Johnson et al. (1990). This figure also shows that the solid volume fraction increases with distance from the wall to a certain maximum in the mid-section. It then decreases and becomes quite small in the saltation region.

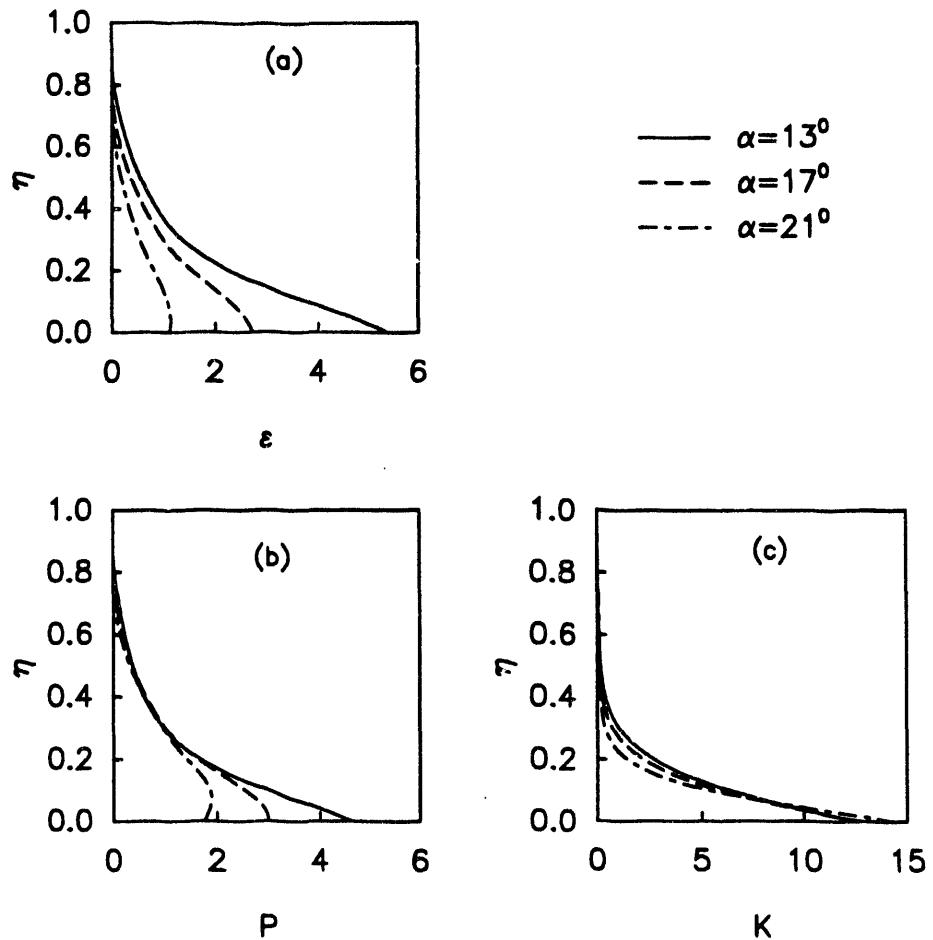


Figure 6. Variations of nondimensional energy dissipation, energy production and fluctuation energy flux for granular over a bumpy chute at different inclination angles.

Variations of the SR-fluctuation kinetic energy,  $w$ , are shown in figure 4c. It is observed that there is a region of large fluctuation kinetic energy near the wall. This is because one main source of the fluctuation energy production is the collisions between particles and wall and occurrence of the slip velocity. Thus, the highest fluctuation energy is found next to the wall.

Away from the wall, the fluctuation kinetic energy generally decreases and reaches to its minimum value at the free surface. Figure 4c also shows that as the inclination angle of the chute increases,  $w$  increases.

For the conditions of figure 4, the variations of non-dimensional normal stress, tangential stress, energy dissipation, energy production, and fluctuation energy flux are shown in figures 5 and 6. Figure 5 shows that the normal and tangential stresses have their highest values at the wall, and their magnitudes decrease with increasing distance from the wall. As the inclination angle increases, the non-dimensional normal and tangential stresses decrease. Figure 6 shows that the energy production, the energy dissipation and the fluctuation energy flux, generally, increase toward the wall. It is also observed that the energy dissipation and production rates decrease as  $\alpha$  increases, while the fluctuation energy flux increases very near the wall and decreases at distances away from the wall. Figures 5 and 6 show the normal and tangential stresses, the energy production and dissipation rates and the fluctuation energy flux are very small in the saltation region.

## TWO-PHASE FLOWS

As was noted in the previous report, a computational model for solving dense and dilute two-phase flows was developed. In this section, the computational model predictions for mean gas velocity, mean particle velocity, and phasic turbulence intensities are presented and compared with the experimental results of Tsuji et al. (1984). In addition, the variations of phasic shear and normal stresses, as well as the phasic fluctuation energy production and dissipation are also evaluated.

Using a Laser-Doppler Velocimeter (LDV), Tsuji et al. reported measurements of the phasic flow properties in a fully developed, two-phase, air-particle turbulent flow in a 30.5 mm

vertical pipe. In their experiments, polystyrene spheres with density of  $\rho_0 = 1020 \text{ kg/m}^3$  and diameters in the range 0.2 mm to 1 mm were suspended in air. A restitution coefficient of  $r = 0.9$ , for particle-particle collisions, and  $r_w = 0.7$ , for particle-wall collisions and a coefficient of dynamic friction  $\mu = 0.2$  between a particle and the wall are used in the present study. These values are consistent with the observation of Govan et al. (1989), who studied the trajectories of glass spheres transported in a small pipe under conditions similar to those of Tsuji et al. (1984).

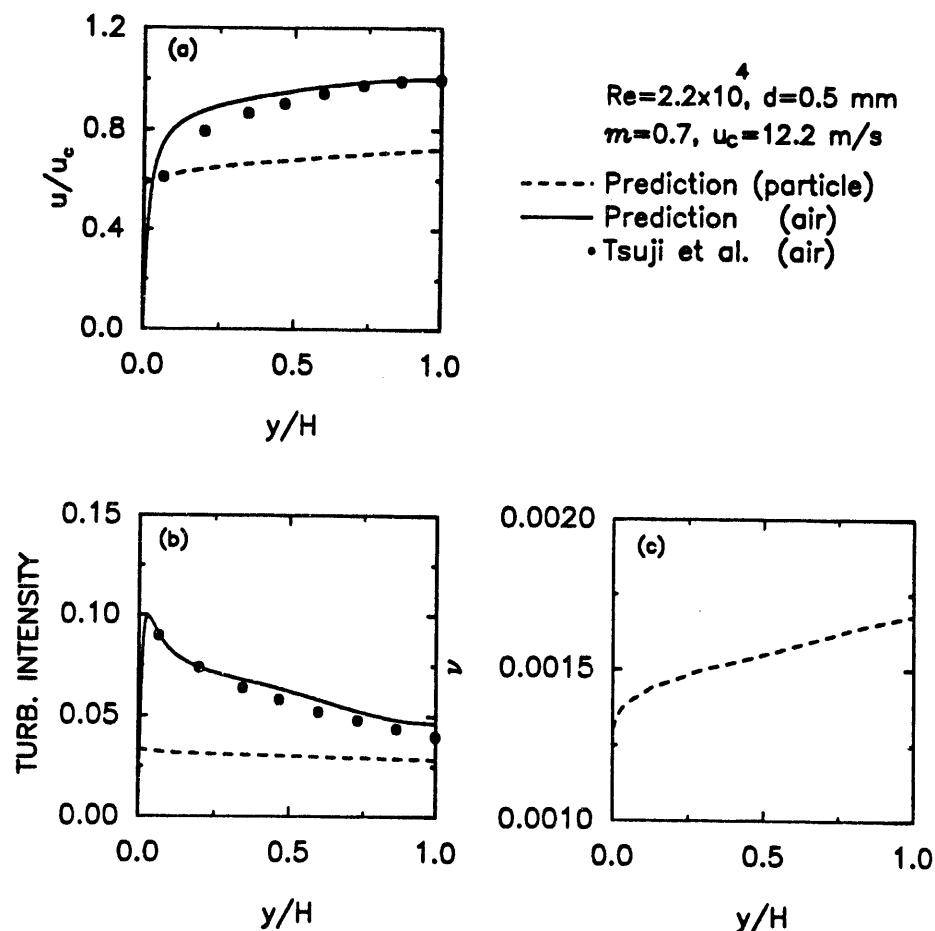


Figure 7. Sample prediction results for two-phase flows in a duct.  
 Comparison with the experimental data of Tsuji et al. (1984).

For a mass loading ratio of 0.7 and a Reynolds number of 22,000, the model predictions

are shown in figure 7. Here the particles are 0.5 mm polystyrene spheres and the flow is upward. Figure 7a shows the mean air and particulate phasic velocities. The effects of presence of particles on the air flow is similar to those reported in the previous report. The presence of particles somewhat flattens the mean air velocity distribution in comparison to the clear gas case. The velocity profile for the particulate phase is relatively flat and shows considerable slip at the wall. The particle mean velocity is also much lower than the gas velocity which is expected for these relatively large and heavy particles in an opposing gravitational field. The experimental data of Tsuji et al. (1984) are also reproduced in this figure for comparison. It is observed that the agreement between the measured and the predicted mean fluid velocities is very good. Unfortunately, experimental data for the mean particulate velocity was not reported for a comparison to be made.

Turbulence intensities of gas and particulate phases are shown in figure 7b. It is observed that the air turbulence intensity is larger than that of the particulate phase. Furthermore, the intensity of air turbulence is increased with the presence of particles when compared with the case of a single phase gas flow. This figure also shows that there is an excellent agreement between the present model predictions and the experimental data for air turbulence intensity. Figure 7c presents the solid volume fraction profile. It is observed that  $\nu$  is of the order of 0.0015 and it is somewhat low near the wall and increases toward the channel centerline.

The model predictions for the variations of stresses in this case are shown in figure 8. Figure 8a shows the phasic normal stress profiles across the duct. It is observed that the normal stress for particulate phase is roughly constant, while the normal stress profile for gas phase has a sharp increase near the wall and then decreases toward the channel centerline. Figure 8a also shows that the normal stress for the gas phase is much larger than that of the particulate phase. Figure 8b shows the shear stress profiles for particulate and gas phases. It is observed that the shear

stress for the gas phase has relative high value at the wall, and decreases to zero at the channel centerline. The shear stress of the particulate phase is very small at the wall, and increases to its maximum value at about 25% of channel half width. It then decreases to zero at the channel centerline. The total normal and shear stresses are presented in figure 8c. It is noticed that the total normal stress has a very sharp peak near the wall region, and decreases gradually toward the channel centerline. The total shear stress has a nearly linear profile with its peak being at the wall.

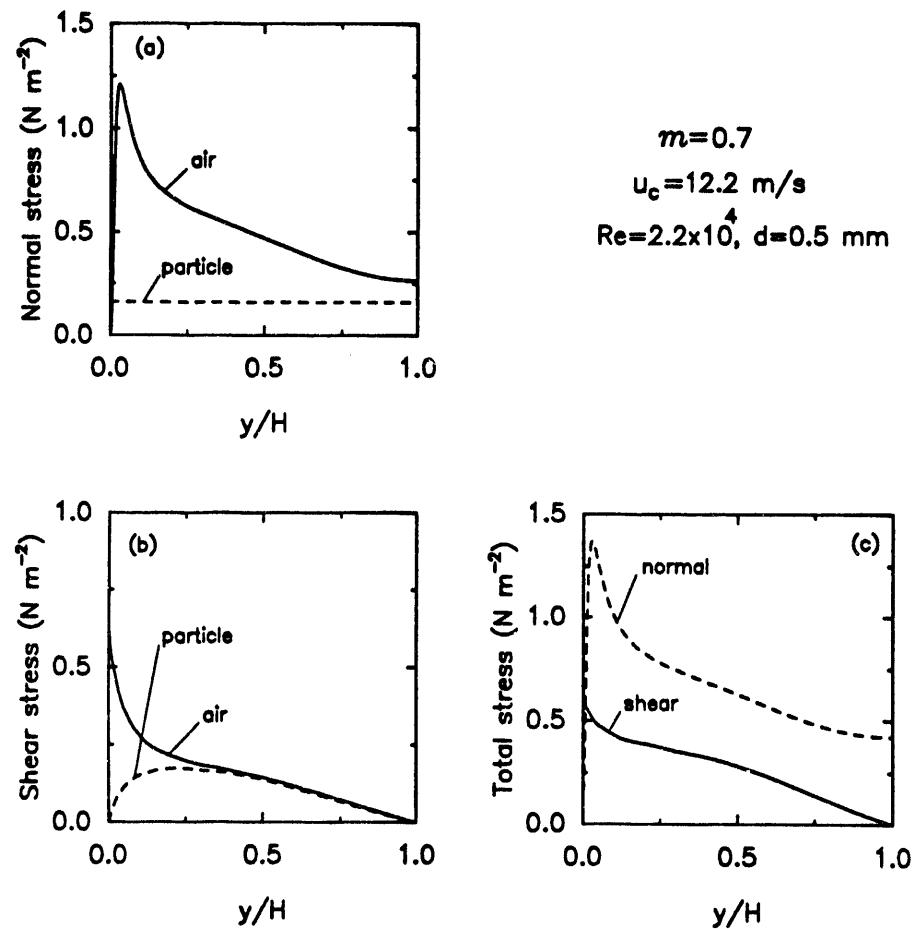


Figure 8. Variation of phasic and total normal and tangential stresses for gas-solid turbulent flows.

Figure 9a presents the variations of the phasic momentum supply terms for particulate

phase and gas phase. This figure indicates that the momentum transfer for particulate phase is negative near the wall, and becomes positive at a very short distance from the wall and increases to about  $175 \text{ N/m}^3$  at the channel centerline. This means that the particles receive momentum from the air in the entire channel except very near wall where they transfer momentum to the air. As expected, the momentum supply term for the air is equal in magnitude and opposite in sign to that of particles. This is because the net phasic momentum transfer must be zero.

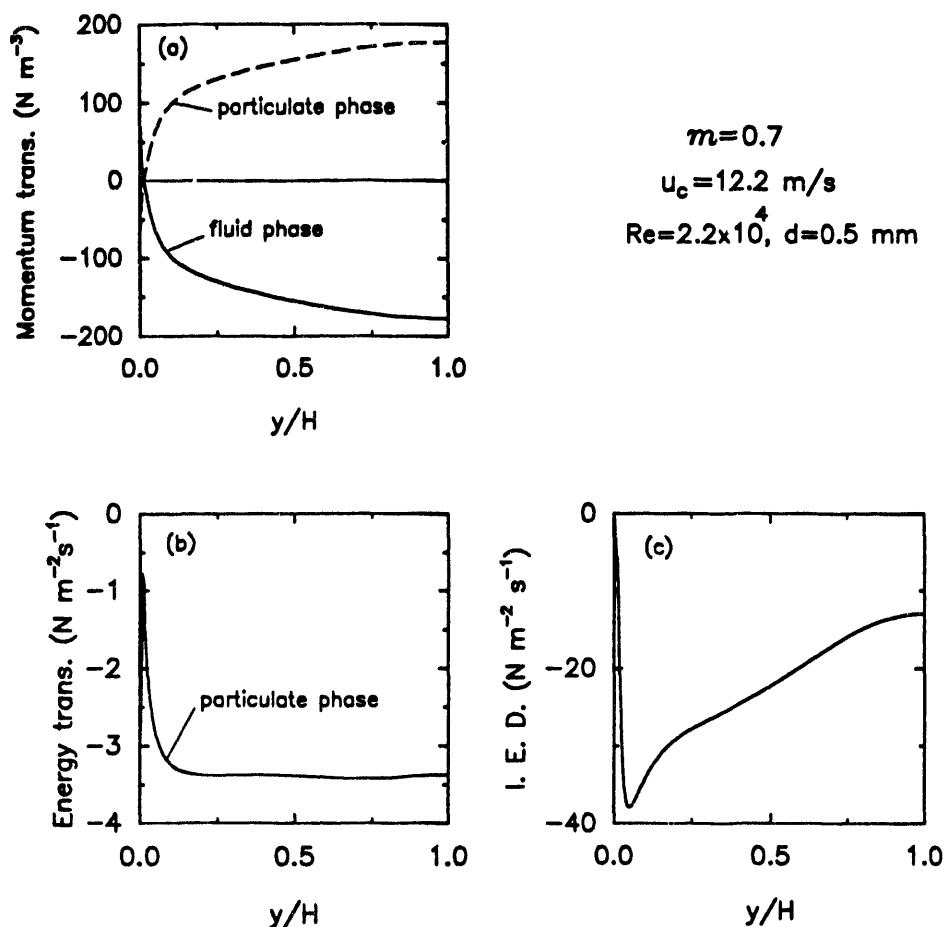


Figure 9. Variation of momentum and energy supply terms and interaction energy dissipation for gas-solid turbulent flows.

The variation of the phase fluctuation energy supply for particulate phase is shown in

figure 9b. It is observed that the energy supply for the particulate phase is negative, which implies that the fluctuation energy is transferred away from the particulate phase. The fluctuation energy supply profile is relatively flat across the channel except for a sharp decrease in magnitude near the wall.

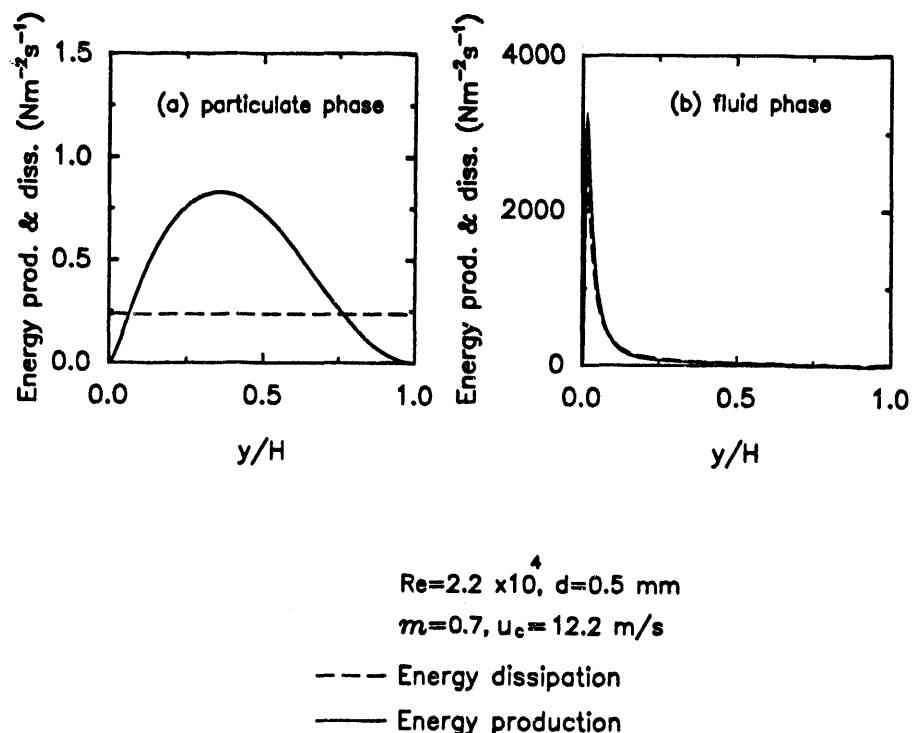


Figure 10. Variations of energy production and dissipation profiles for gas-solid turbulent flows.

It should be emphasized that the fluctuation energy interaction process involve significant amount of energy dissipation. The net interaction energy is always negative indicating a loss of energy. Variation of the interaction energy dissipation profile is shown in figure 9c. It is

observed that the magnitude of the energy interaction dissipation reaches to its maximum near the wall, and then decreases gradually toward the channel centerline.

The energy dissipation and production profiles for particulate and fluid phases are shown in figure 10. Figure 10a shows that the particulate energy dissipation is roughly constant across the flow region and it is generally less than the energy production rate except in the neighborhood of the wall and the channel centerline. The particulate energy production is zero at the wall and at the centerline, and reaches to its peak value at the distance of about one-third of half-width of the channel from the wall. Figure 10a also shows that the net production of fluctuation energy exceeds the dissipation rate. Part of the excess energy is transferred to the fluid phase and the other part is consumed by the interaction energy dissipation. Figure 10b shows that the fluid phasic energy production and dissipation have sharp peaks near the wall, and decrease rapidly toward the channel centerline. These characteristic are typical of clear gas turbulence. From this figure, it is also observed that the energy production is somewhat larger than the dissipation rate. The excess fluctuation energy production balances the interaction fluctuation energy dissipation.

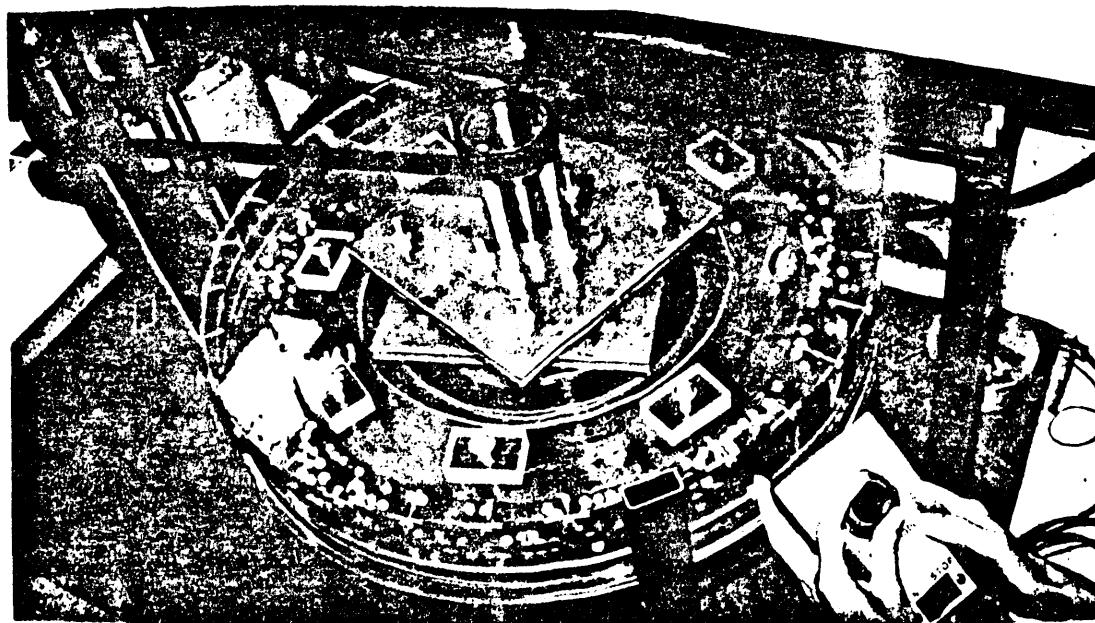


Figure 11. Experimental mono-granular shear flow setup.

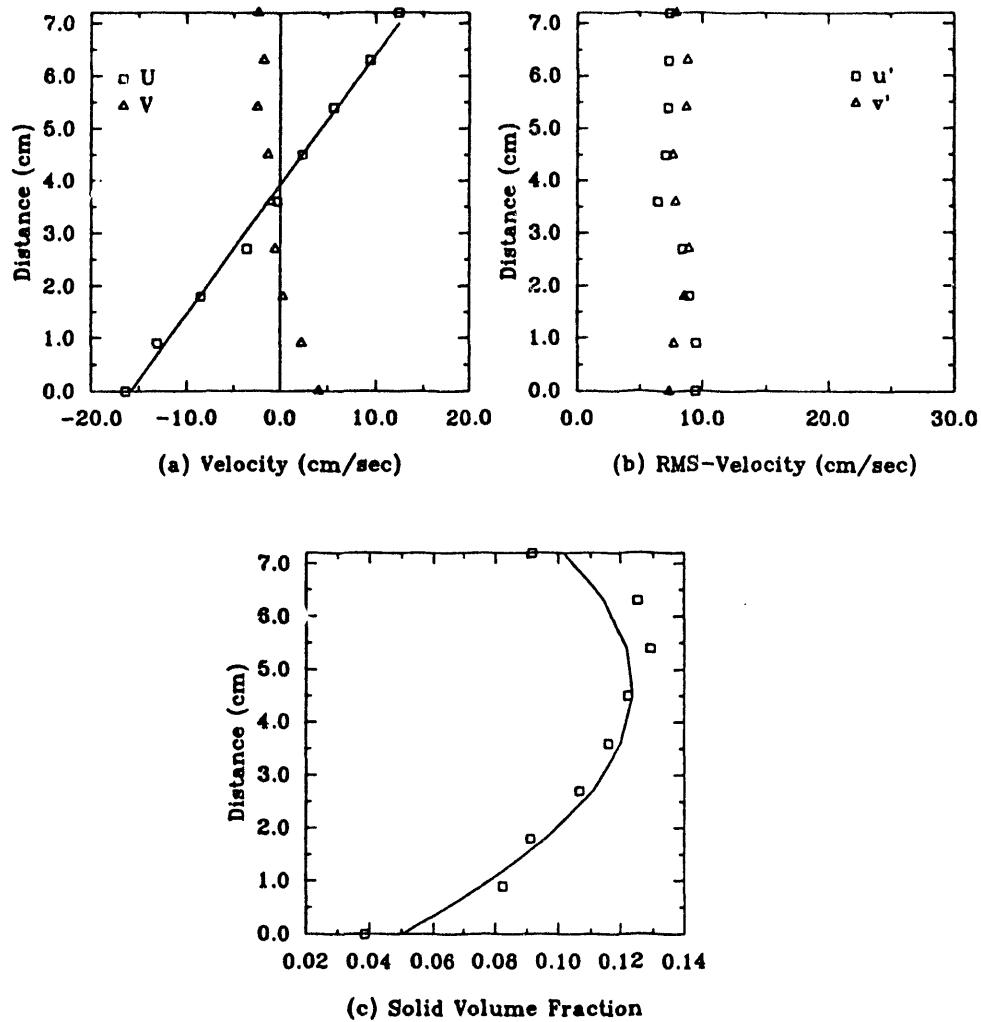


Figure 12. Experimental data for mean velocity, RMS-fluctuation velocities, and solid volume fraction.

## EXPERIMENTAL STUDY

A mono-granular simple shear flow setup was constructed and was used for the experimental study. A collection of multi-colored spherical glass balls which are 12 mm in diameter were used as granular particles. A picture of the setup is shown in figure 11. A video camera is used to record the motions of particles. For different shear rates, the position of the balls in consecutive frames taken 1/30th of a second apart were measured. Using this technique, the velocity vector of each particle was calculated. The shearing region was divided into 10-15

equivalent horizontal segments. Averaging procedures are used to provide the experimental velocity and concentration profiles.

Figure 12 show sample experimental data for mean velocity, concentration and fluctuation velocity profiles for a mean solid volume fraction of 9.8% and a shear rate of  $4\text{s}^{-1}$ . It is observed that the significant amount of slip exist. The slip is much larger at the inner wall when compared with that of the outer wall. Figure 12a also shows that the axial velocity is roughly linear in shearing region. From figure 12b it is observed that the fluctuation energy components are roughly constants, while the solid volume fraction varies across the section with a peak near the centerline of the shear cell.

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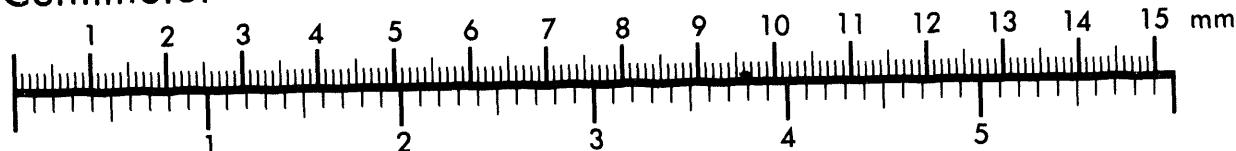
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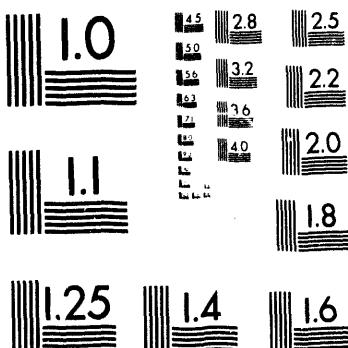
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