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**Quarterly Technical Progress Report**

(June 1, 1993 to August 31, 1993)

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

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

**Goodarz Ahmadi**

**Department of Mechanical and Aeronautical Engineering**

**Clarkson University**

**Submitted to**

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**Pittsburgh Energy Technology Center**

**Attention:**

**Dr. Mehrdad Massoudi**

**Project Officer**

**MASTER**

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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 June 1, 1993 to Aug 31, 1993, the thermodynamically consistent, rate dependent model for turbulent two-phase flows analysis was used and the phasic fluctuation energy dissipation rates are evaluated. Further progress on the application of the kinetic model for rapid flows of granular materials including the frictional energy losses were made. The velocity, the fluctuation energy and the solid volume fraction profiles for granular flows down a vertical channel were obtained. The results were compared with the molecular dynamic simulations of Savage and good agreement was obtained.

The computational model was used and the rapid granular flows around a rectangular block in a channel were analyzed. It is shown that the model is capable of predicting the features of the flows in complex geometries. The evaluated profiles for solid volume fraction and fluctuation energy show the expected trend of variations. The effect of bumpy wall on flow of granular materials was analyzed. The special case of Couette flow was studied. The preliminary results obtained is quite encouraging.

Further progress was made in the experimental study of mono-layer simple shear flow device. Preliminary data concerning the shearing of 12 mm multi-color glass particles are obtained. The preliminary experimental data for the solid volume fraction shows the expected variation.

## **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 nonreacting turbulent flows of dense or dilute multiphase coal mixtures will be provided.

## HIGHLIGHT OF THE EARLIER ACCOMPLISHMENTS

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.

The computational model for rapid granular and two-phase flows in complex geometries was further 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 simulation results of Campbell and Brennen, and good agreements were observed. Progress has been made in developing an appropriate computational model for analyzing turbulent two-phase flows with various loadings.

An experimental setup for generating simple shear flows of a mono-granular layer was constructed. Sample results for shearing of 12 mm multi-color glass particles was obtained.

## A THERMODYNAMICALLY CONSISTENT RATE-DEPENDENT MODEL FOR TURBULENT TWO-PHASE FLOWS

A thermodynamically consistent theory for dense two-phase flow was developed. The new model includes the transport equations for the phasic fluctuation kinetic energies. Anisotropic and rate-dependent expressions for the phasic stress tensors were derived. For dense solid-liquid mixtures, the material parameters of the model were evaluated from the limiting conditions. The special case of simple shear flows of glass beads-water mixtures were studied. The coefficient of restitution for glass bead collision in water was experimentally measured and used in the model predictions.

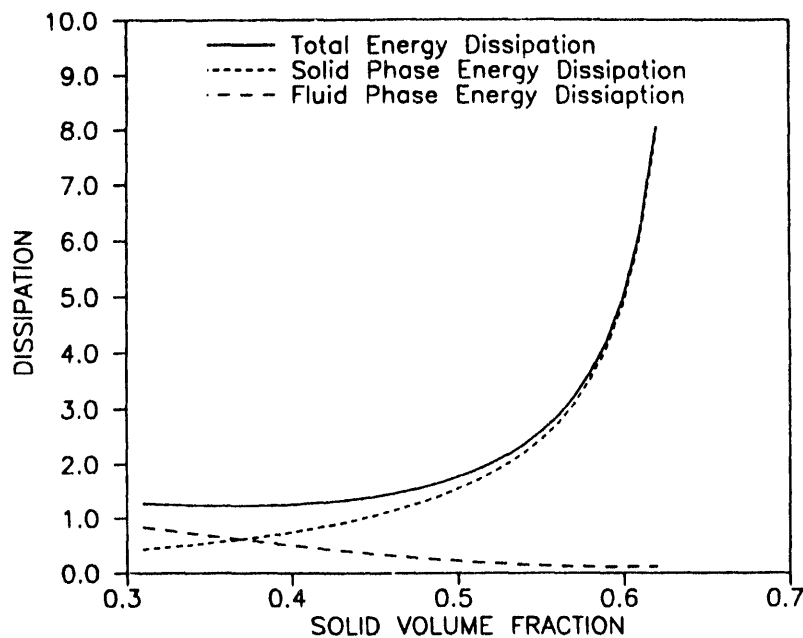


Figure 1. Variations of nondimensional phasic fluctuation energy dissipation with solid volume fraction for 1.1 mm glass beads in water.

Unlike the available models, the new rate-dependent formulation is capable of predicting the production and dissipation rates of phasic fluctuation energies. Figure 1 shows

variations of nondimensional phasic fluctuation energy dissipation with solid volume fraction for a mixture of 1.1 mm glass beads in water. It is observed that the nondimensional particulate fluctuation energy dissipation increases rapidly with an increase in solid volume fraction. The fluid fluctuation energy dissipation, however, decreases as  $v$  increases. For the present condition, the phasic fluctuation energy dissipation rates become equal for a  $v$  of about 0.35. This figure shows that for large solid volume fractions, the fluctuation energy is mainly dissipated by the particulate phase and the contribution of the fluid phase is negligible as  $v$  approaches the limiting maximum solid volume fraction of about 0.64. The dissipation rate of the fluctuation energy also becomes extremely large close to the maximum packing conditions. For smaller values of  $v$ , the fluid phasic energy dissipation become rather large and that of the solid phase decreases. Experimental confirmation of these results is not possible at the present time due to the lack of data for the phasic fluctuation energy production. However, the predicted trends of variation seems reasonable.

## **ANALYSIS OF RAPID GRANULAR FLOWS INCLUDING FRICTIONAL LOSSES**

The kinetic model for particulate flows, including frictional energy losses, was used to analyze the rapid granular gravity flows down a vertical channel. The equations of motion were solved using a fourth-order Runge-Kutta numerical scheme. The corresponding mean velocity and solid volume fraction profiles are shown in figure 2. The data of Savage (1979) is also shown in this figure for comparison. It is observed that the predicted roughly paraboloidal mean velocity profile is in good agreement with data of Savage. Figure 2 also shows that the fluctuation energy has a rather high value in the shearing region near the wall, and decreases to its minimum value near the centerline. The solid volume fraction has an opposite trend of variation. It has a somewhat low value near the wall, and increases to its peak value near the centerline.

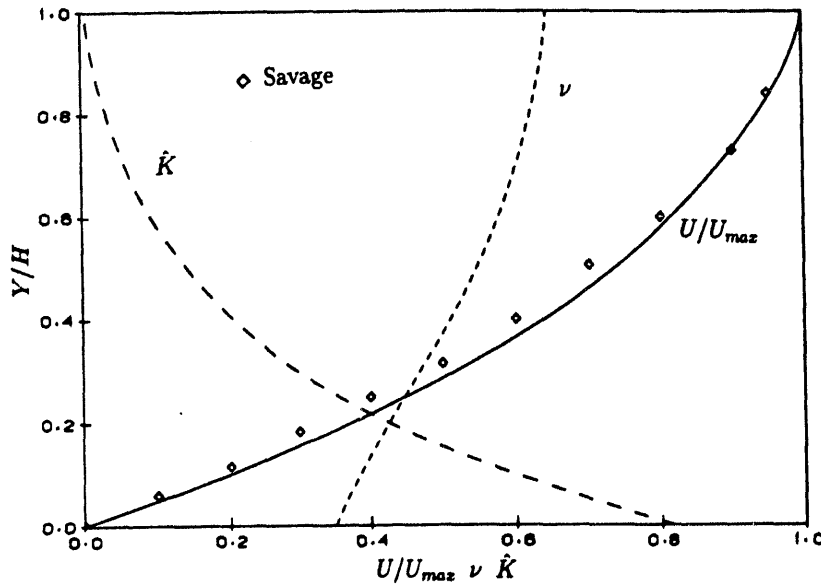


Figure 2. Variations of mean velocity, fluctuation energy, and solid volume fraction profiles for granular flows down a vertical channel. Comparison with the data of Savage (1979).

## 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 Around a Block

Progress was made in application of the computational model to granular flow analysis in nonsimple regions. The special case of granular flow around a rectangular cylindrical block in a channel was studied in details. As was described in the earlier report, the flow region was assumed to be 15 m long and 2.4 m wide. The flowing granular layer thickness was taken to be about 0.25 m. A 1.5 m long, 0.8 m wide and 0.25 m high rectangular block was assumed to be

located at the center of the channel. The physical properties of spherical polystyrene beads with a specific gravity of 1.03 and the mean diameter of approximately 1.2 mm were used in the simulation.

The details of the discretization were described in the earlier report.

Accordingly, a uniform rectangular grid system with 30 elements along the x-direction, 24 elements along the y-direction, and eight element in the z-direction were used. The length increments of  $\Delta x=0.5$  m and  $\Delta y=0.1$  m were used. A total of 5760 elements was used to represent the granular flow region. The computed results shows that the flow around the block involves a rather complicated accelerating and decelerating zones.

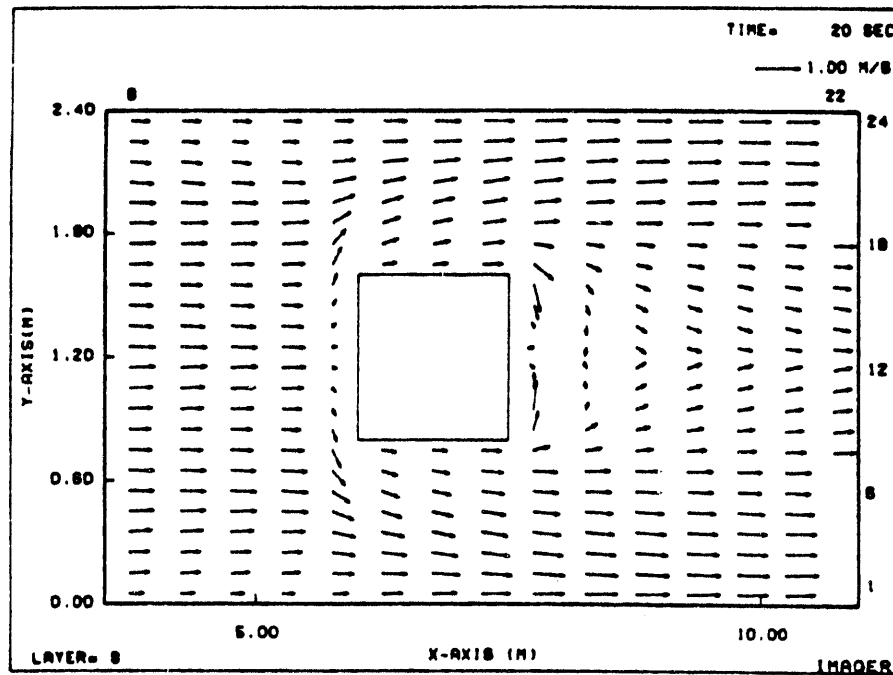


Figure 3. Velocity vector plot at the surface layer in the (x, y) plane at t=20 sec.

Several computer simulation results were shown in earlier reports. Closeup of the velocity fields are shown in Figures 3 and 4. These figures, respectively, show the velocity vector

plot in top layer of the (x, y) plane of the flow region at times of  $t=20$  and  $t=30$  sec. It is observed that the block significantly distorts the flow field. In particular, on both sides of the block, the flow accelerates and a separation bubble is formed behind the block. At the center line behind the block a sink flow seems to appear. Further downstream, the wake region can be seen. Comparison of figures 3 and 4 shows that the flow has reached the steady state conditions after about 20 sec.

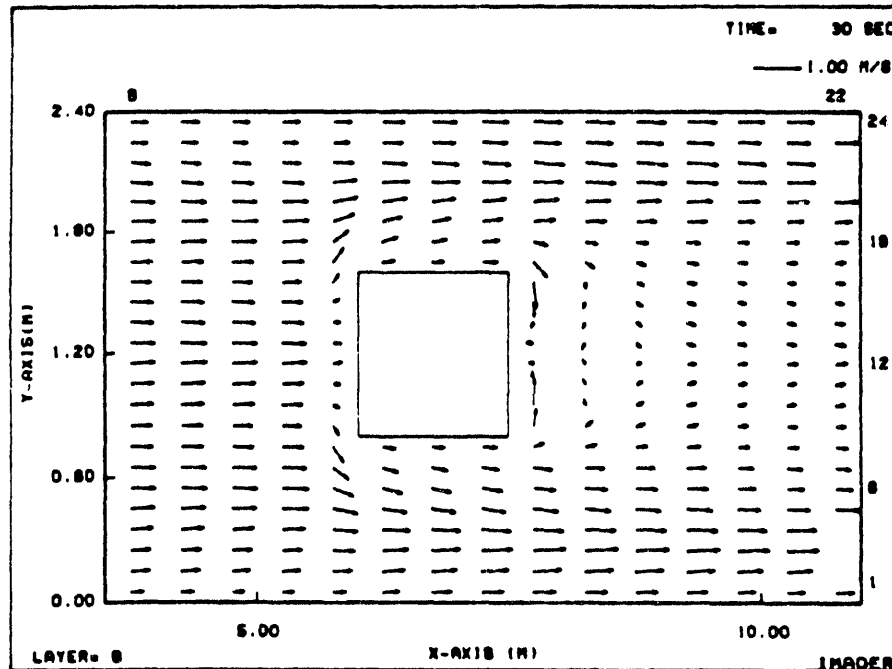


Figure 4. Velocity vector plot at the surface layer in the (x, y) plane at  $t=30$  sec.

Figure 5 shows the solid volume fraction profiles for different sections in the plane of symmetry of the flow region at time  $t=10$ sec. It is observed that away from the block (AB) the solid volume fraction increases with depth. In front of the block (FB), the solid volume fraction does not change appreciably. Behind the block (BB), however, the particles seem to pile up and the solid volume fraction increases significantly and approaches its limiting maximum value of about 0.64.

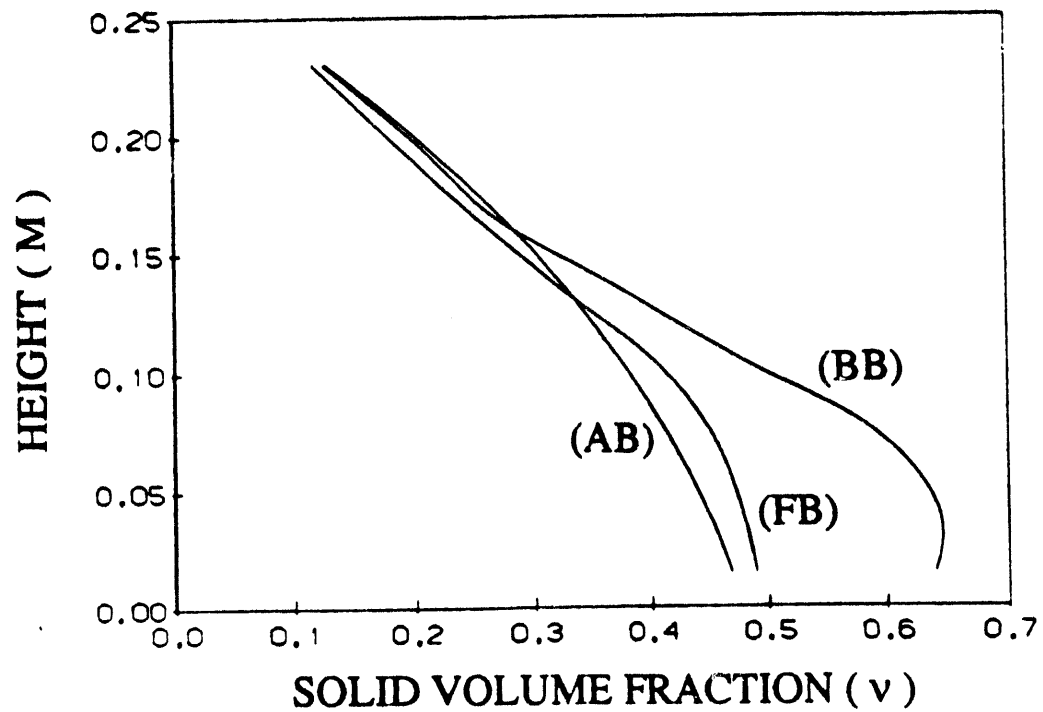


Figure 5. Solid volume fraction profiles at different sections at  $t=10$  sec.

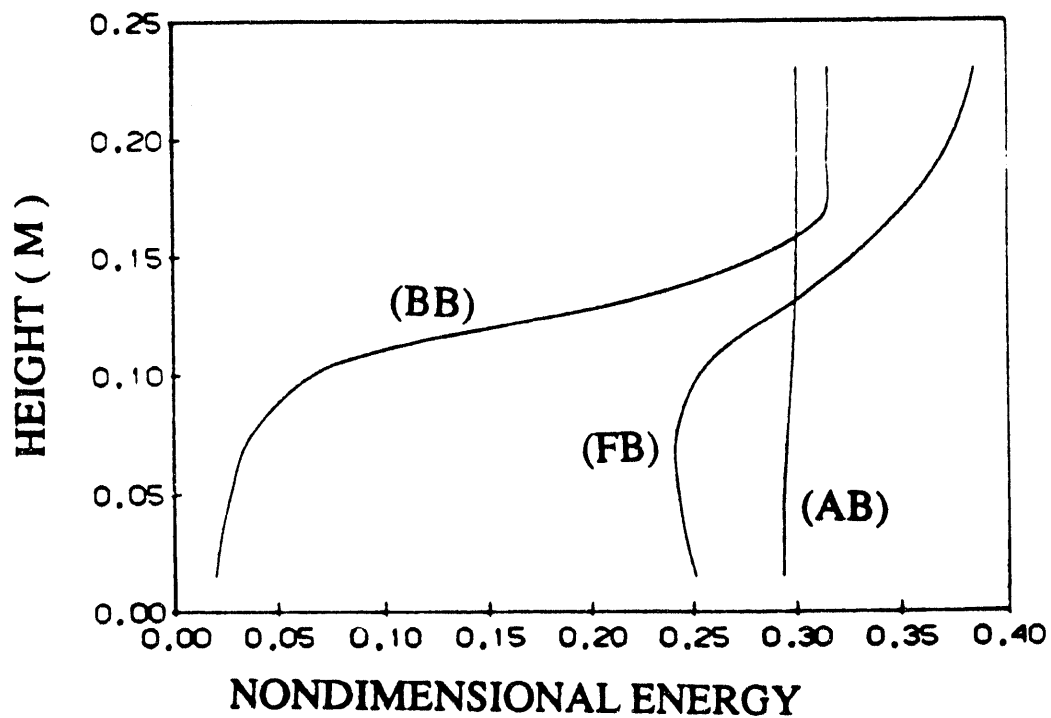


Figure 6. Fluctuation energy profiles at different sections at  $t=10$  sec.

In Figure 6, variations of fluctuation energy profiles at different section in the plane of symmetry at time  $t=10\text{sec}$  are shown. It is observed that away from the block (AB) the fluctuation energy remains almost uniform independent of depth. In front of the block (FB), the fluctuation energy increases near the free surface and decreases near the bottom layer. The fluctuation energy decreases significantly with depth and becomes quite small near the bottom of the channel.

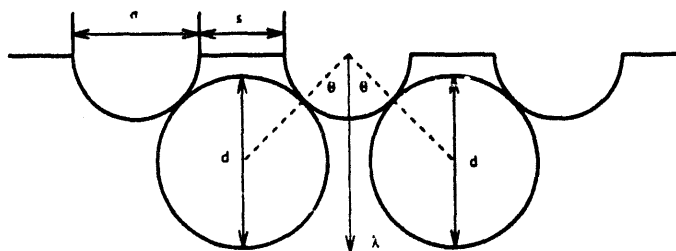


Figure 7. Schematics of a bumpy wall.

### Granular Flows with Bumpy Boundary

The interactions of particle with the boundary is known to significantly affect flow and transport of granular materials. The schematics of a bumpy boundary is shown in figure 7. The kinetic model of granular materials including frictional losses was used in the analysis. The presence of bumpy boundary conditions leads to a strongly couple system of governing equations which has to be solve numerically even for simple case of Couette flow. A special discretization scheme was developed and the mean velocity, the fluctuation kinetic energy and the solid volume fraction profiles for granular flows between two parallel was were evaluated. The results for different values of friction coefficients are plotted in figure 8. The molecular dynamic simulation results of Savage and Dai (1992) for the frictionless particles are also shown in this figure

for comparison. It is observed that the model predictions are in excellent agreement with the molecular dynamic simulation results.

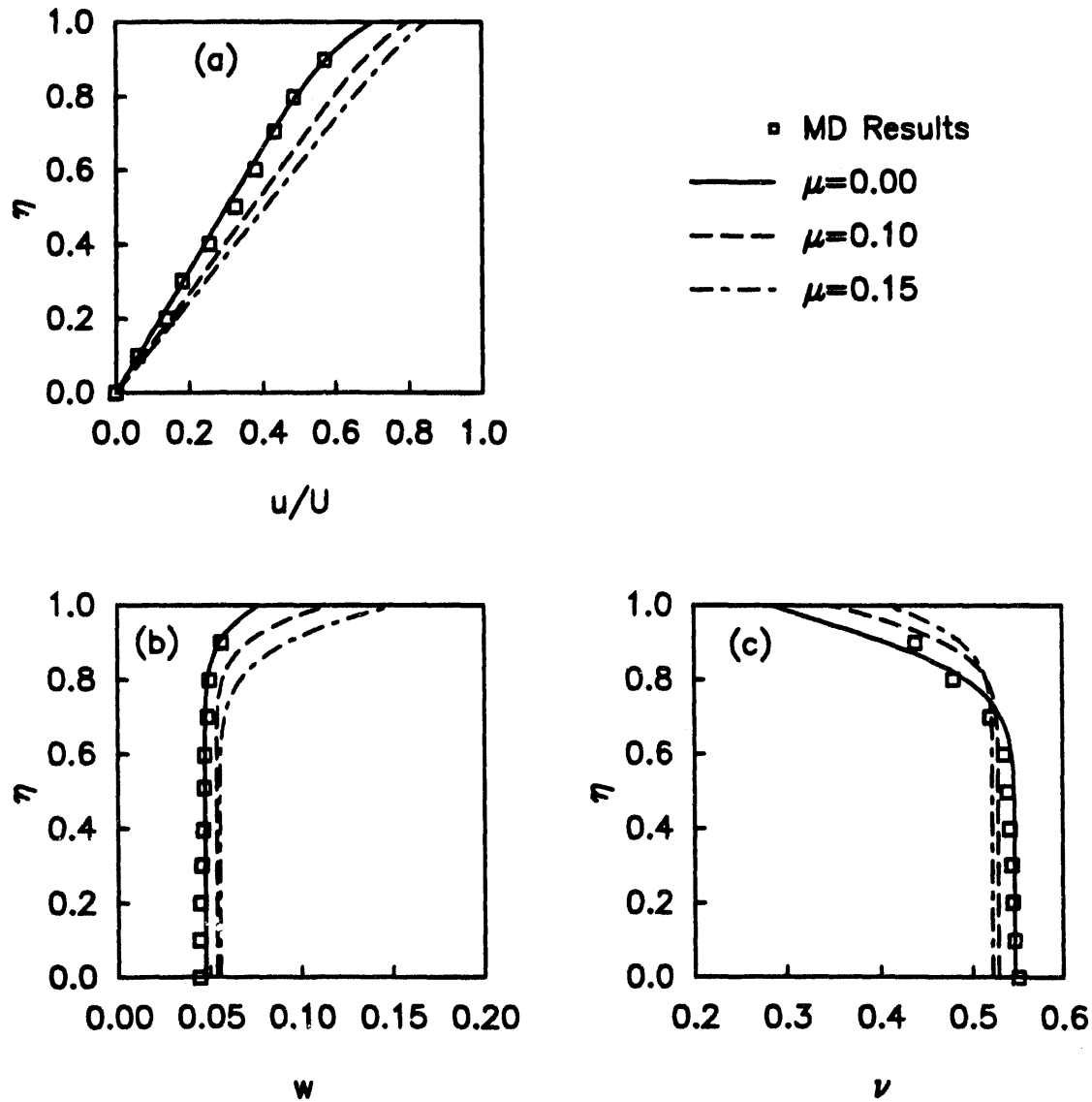


Figure 8. Variations of mean velocity, fluctuation energy and solid volume fraction profiles. Comparison with the molecular dynamic simulation of Savage and Dai (1992).

Figure 8a show that there are a significant amount of slip at the wall. The slip velocity decreases as the friction coefficient increases. Figure 8b indicates that the fluctuation velocity is rather large near the wall and approaches a constant away from the wall. The solid volume fraction, on the other hand, is small near the wall and increases with distance from the wall.

Figure 8c shows that  $v$  is roughly constant in the core region. These results show that the commonly used assumptions of a linear mean velocity and constants values of kinetic energy and solid volume fraction for Couette flow of granular materials are not correct.

### **Two-Phase Flow**

Formulation of appropriate equations for motion of dense two-phase mixtures, and some features of the computational scheme of solution were described in the earlier report. Effort has been made to include the effects of fluid turbulence, particles fluctuation energy and collisional stresses into the computational model. The suitability of different boundary conditions for the fluid phase and particulate phase are also studied.

## **EXPERIMENTAL STUDY**

The main objective of the experimental effort is to provide a fundamental understanding of the mechanisms that control the features of granular particulate flows. The other main goal is to provide reliable data for velocity, concentration and fluctuation energy profiles for a simple shear flow of granular materials in order to verify the foundation of the thermodynamical formulation and computational predictions.

### **Granular Shear Flow Device**

The mono-granular simple shear flow setup with multi-colored spherical glass balls which are 12 mm in diameter were used for the experimental study. Figure 9 shows the schematic of the device and the shearing cell. As was described in the earlier report, the position of the balls in consecutive frames taken 1/30th of a second apart from the test run at a shear rate of 62.83 1/sec were measured. Using this technique, the velocity vector of each particle can be calculated. The shearing region was divided into 10-15 equivalent horizontal segments.

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

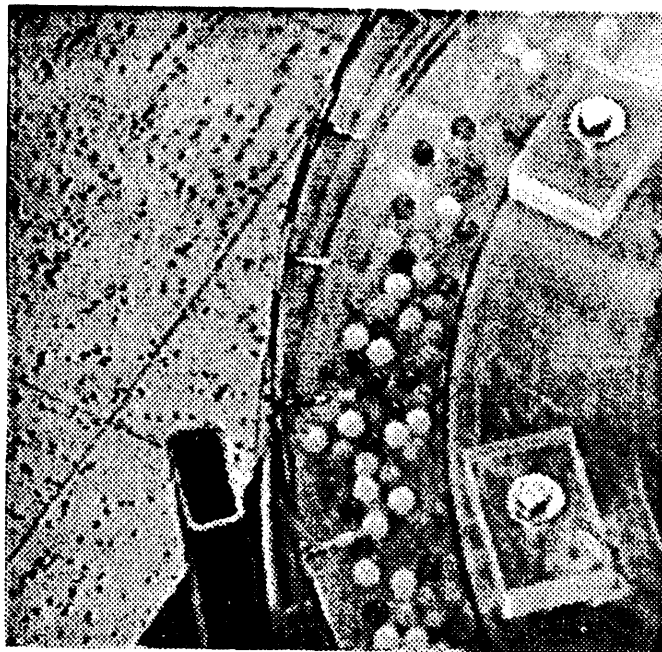


Figure 9. A picture of the simple shear flow device.

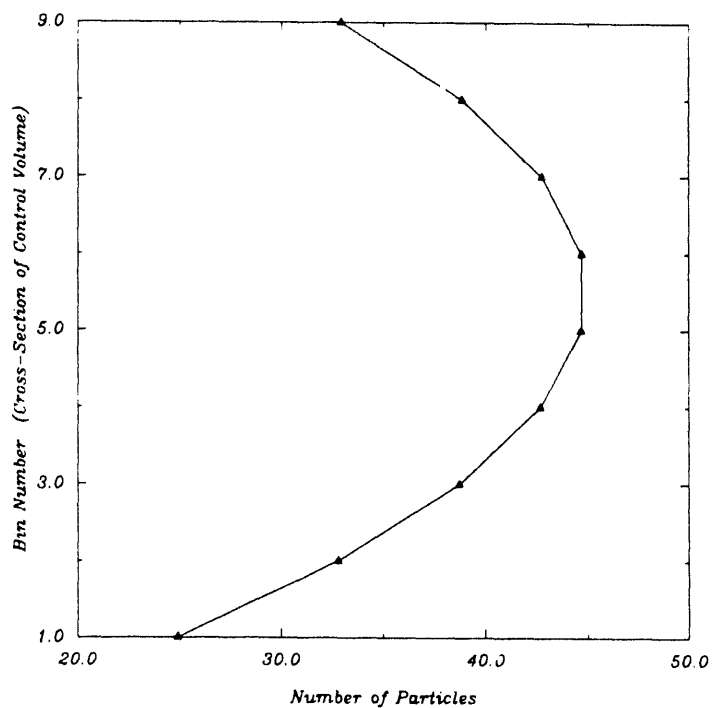


Figure 10. Preliminary experimental data for the solid volume fraction profile.

A sample axial and lateral velocity profiles were presented in the earlier report. Figure 10 shows a sample concentration profile. It is observed that the solid volume varies significantly across the section. It is quite low near the walls and relative high in the core region. This variation is in qualitative agreement with our numerical simulation results for a simple Couette flow as shown in Figure 8c. Figure 10, however, shows that the concentration near the outer wall is lower than that near the inner wall. This trend is opposite to the effect of the centrifugal force which pushes the particle toward the outer wall.

## **ARTICLES AND PRESENTATIONS**

### **Journals Publications**

G. Ahmadi and S.J. Chowdhury, "A Rate-Dependent Algebraic Stress Model for Turbulence," *Applied Math. Modelling* 15, 516-524 (1991).

H. Ounis and G. Ahmadi, "Motions of Small Particles in a Turbulent Simple Shear Flow Field Under Microgravity Condition," *Physics of Fluids A* 3, 2559-2570 (1991).

S. Abu-Zaid and G. Ahmadi, "A Thermodynamically Consistent Stress Transport Model for Rotating Turbulent Flows," *Geophys. Astrophys. Fluid Dynamics* 61, 109-121 (1991).

G. Ahmadi, "A Thermodynamically Consistent Rate-Dependent Model for Turbulence, Part I - Formulation," *Int. J. Non-Linear Mech.* 26, 595-607 (1991).

K.A. Elrais, W. Eckerle, G. Ahmadi and A.H. Eraslan, "Simulation of Transient Three-Dimensional Natural Convection and Saturated Pool Boiling, *Int. J. Numerical Methods Heat Fluid Flow* 2, 139-154 (1992).

S.J. Chowdhury and G. Ahmadi, "A Thermodynamically Consistent Rate-Dependent Model for

Turbulence, Part II - Numerical Results," Int. J. Non-Linear Mech. 27, 705-718 (1992).

W.G. Paff and G. Ahmadi, "On Convergence of Karhunen-Loeve Series Expansion for a Brownian Particle," J. Appl. Mech. Trans. ASME (In Press).

S. Abu-Zaid and G. Ahmadi, "A Stress Transport Model for Granular Flows in a Rotating Frame, Int. J. Engng. Sci. 30, 1483-1495 (1992).

S.J. Chowdhury and G. Ahmadi, "Analysis of A Mixing Layer by a Rate-Dependent Turbulence Model," ASCE, Journal of Engineering Mechanics 119, 1700-1706 (1993).

D. Ma, A.H. Eraslan and G. Ahmadi, "A Computer Code for Analyzing Transient Three-Dimensional Rapid Granular Flows in Complex Geometries, Computer Fluids (In Press).

S. Abu-Zaid and G. Ahmadi, "Analysis of Rapid Shear Flows of Granular Materials by a Kinetic Model Including Frictional Losses," Powder Technology (In Press).

### **Conference Presentations**

G. Ahmadi and S. Abu-Zaid, "Overview of Thermodynamical Approach to Modeling Turbulent Flows of Two-Phase Solid-Liquid Mixtures," International Conference on Multiphase Flow '91-Tsukuba, Tsukuba, Japan, September 24-27, 1991.

G. Ahmadi and S. Abu-Zaid, "A Thermodynamically Consistent Model for Turbulent Two-Phase Flows," 28th Annual Technical Meeting of the Society of Engineering Science, Gainesville, FL, November 6-8, 1991.

G. Ahmadi and S. Abu-Zaid, "Analysis of Rapid Shear Flows of Granular Materials by a Stress Transport Model," 28th Annual Technical Meeting of the Society of Engineering Science,

Gainesville, FL, November 6-8, 1991.

G. Ahmadi, "Overview of Thermodynamical Modeling of Turbulent Flows of Multiphase Mixtures," Proceedings of the International Conference on Engineering Application of Mechanics, Vol. 3, Sharif University of Technology, Ed. by M.S. Sadeghipour et al., June 9-12, 1992, 386-399.

G. Ahmadi and S. Abu-Zaid, "A Thermodynamically Consistent Stress Transport Model for Rapid Granular Flows," The 23rd Annual Meeting of the Fine Particle Society, Las Vegas, Nevada, July 13-17, 1992.

G. Ahmadi and S. Abu-Zaid, "A Model for Turbulent Two-Phase Flows," MEET'N'93, ASME/ASCE/SES Joint Meeting, University of Virginia, Charlottesville, VA, June 6-9, 1993.

G. Ahmadi, D. Ma, and A. Eraslan "Rapid Granular Flow in Complex Geometry Regions," MEET'N'93, ASME/ASCE/SES Joint Meeting, University of Virginia, Charlottesville, VA, June 6-9, 1993.

G. Ahmadi, "A Computational Model for Coal Transport and Combustion," University Coal Research Contractors" Review Conference, Pittsburgh, PA, June 23-25, 1993.

G. Ahmadi and S. Abu-Zaid, "Turbulent Two-Phase Flow of Dense Mixtures-A Thermodynamically Consistent Model," The 24th Annual Meeting of the Fine Particle Society and First International Conference on Pharmaceutical Sciences and Technology, Chicago, Illinois, August 23-28, 1993.

J. Cao, and G. Ahmadi, "Numerical Simulation of Granular Couette Flows Between Two Rough Parallel Plates," The 24th Annual Meeting of the Fine Particle Society and First International Conference on Pharmaceutical Sciences and Technology, Chicago, Illinois, August 23-28, 1993.

G. Ahmadi, D. Ma, and A. Eraslan "Analysis of Transient Rapid Granular Flows in a Channel with

**an Obstruction," The 24th Annual Meeting of the Fine Particle Society and First International Conference on Pharmaceutical Sciences and Technology, Chicago, Illinois, August 23-28, 1993.**

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